PACE

PARTNERSHIP TO ADVANCE COMBUSTION ENGINES

Fuel Injection and Spray Research

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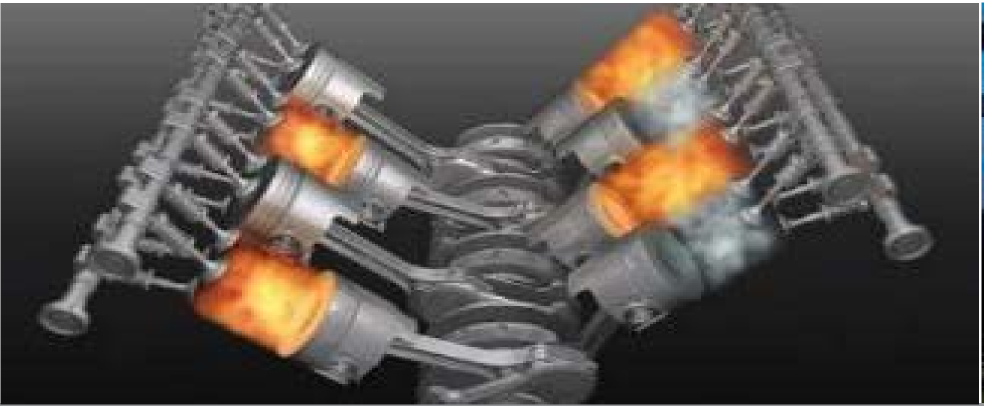
Annual Merit Review, 2 June 2020

Project ACE143



U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

Overview: Experiments and Simulations of Injection and Sprays

- **Timeline**
  - All projects started mid-2019
  - Projects end in 2023, 25% complete

- **Budget**

Task	Description	FY19	FY20
D.01.01 Powell	Argonne, Free spray and wall film x-ray experiments Powell, Sforzo, Tekawade	$200k	$200k
D.01.02 Wissink	ORNL, Wall temperature and film neutron-scattering experiments; Wissink	$47k	$200k
D.01.03 Nguyen	SNL, Evaporative free spray and soot film combustion modeling; Nguyen, Tagliente, Pickett, Chen	$100k	$100k
D.01.05 Pickett	SNL, Free spray and wall film optical experiments Pickett, Skeen, Manin, Hwang, Cenker, Maes	$380	$380
D.02.01 Torelli	ANL, GDI spray wall interaction modeling Torelli, Som	$300k	$300k
D.02.02 Waters	LANL, Free spray and wall impingement, including VOF Waters, Carrington	$200	$200

Budgets above reflect each project's total for PACE, rather than the share of the work discussed in this presentation

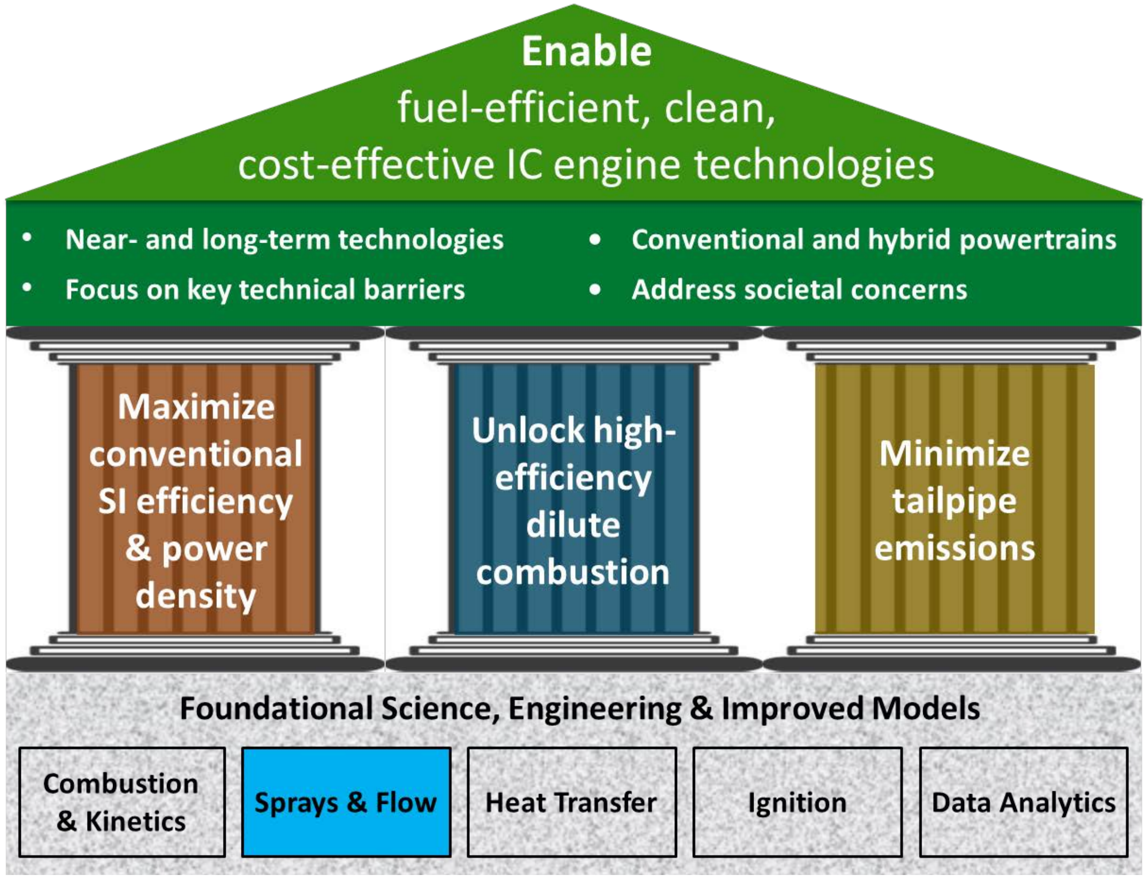
- **Barriers**
  - Ability to predict and mitigate knock and pre-ignition at high load
  - Overcome barriers to lean/dilute combustion
  - Enable zero-impact tailpipe emissions
  - Need for accurate fuel spray submodels.
  - Inadequate understanding of the fundamentals of fuel injection

- **Partners**
  - PACE, a DOE-funded consortium of 6 National Laboratories working towards a common goal
  - PACE sprays team coordinates tasks and sets direction
  - 15 Industry partners in the AEC MOU.
  - Engine Combustion Network, Spray G (20+ partners)
  - CONVERGE Working Group: Universities, Labs, Convergent Science Inc

Relevance: Major Outcomes of PACE and the Role of the Sprays Team

Improved understanding and modeling of sprays, films, and mixture formation addresses

- **Ability to Predict and Mitigate Knock and Pre-ignition at High Load**
  - Simulation and experiments characterizing free sprays, wall impingement, and mixture formation
- **Overcome Barriers to Lean/Dilute Combustion**
  - Measurements and modeling of mixture formation under lean/dilute conditions
  - Measure and model spray variability
- **Minimize tailpipe emissions**
  - Experiments and modeling including multiple injections at cold-start conditions
  - Modeling of spray-wall interactions, films, vaporization, heat transfer, wall-film soot
  - How to create a combustible mixture at the spark plug on Cycle 1?



Milestones, FY2019 and FY2020 (1)

Month / Year	Task	Description of Milestone or Go/No-Go Decision	Status
Sep 2019	D.02.01 Torelli	Validation of recently developed spray-wall interaction model against x-ray measurements under GDI G2, G3 conditions	75%
Nov 2019	D.01.05 Pickett	Share free-spray dataset on time-resolved 3D liquid volume fraction at eleven conditions	Complete
Dec 2019	D.01.03 Nguyen	Model implementation and validation for both Diesel and Gasoline injection	Complete
Dec 2019	D.02.02 Waters	Validate the single injection gasoline cases with current mode	Complete
Mar 2020	D.02.01 Torelli	Validation of recently developed spray-wall interaction model against x-ray measurements under GDI cold-start conditions	75%

Milestones, FY2019 and FY2020 (2)

Month / Year	Task	Description of Milestone or Go/No-Go Decision	Status
Mar 2020	D.01.03 Nguyen	Multi-component free spray simulation under various conditions	75%
Mar 2020	D.01.01 Powell	Submit measurements results to the 7th ECN Workshop for comparison with simulation predictions	Complete
June 2020	D.01.02 Wissink	Complete imaging campaign of Spray G internal dynamics at G3 conditions and share results with ECN.	On track
July 2020	D.01.05 Pickett	Free-spray experiments using chosen PACE (7-9 component) surrogate	On track
Sep 2020	D.02.02 Waters	Improve the evaporation model for free spray heat and mass transfer and validate the iso–octane cases	On track
Sep 2020	D.01.01 Powell	Dataset of measurement results including free-spray and wall-film measurements will be archived online.	On track

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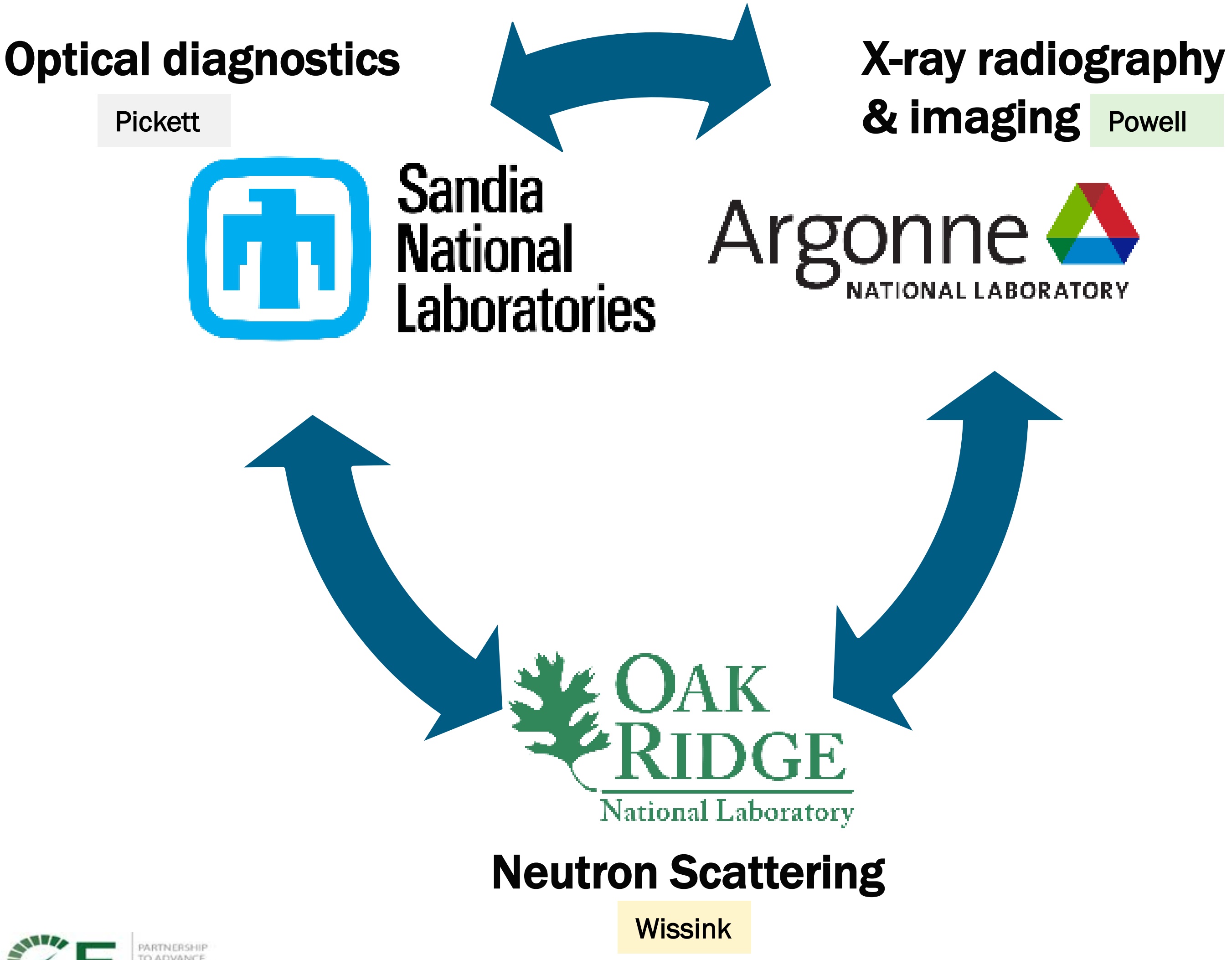
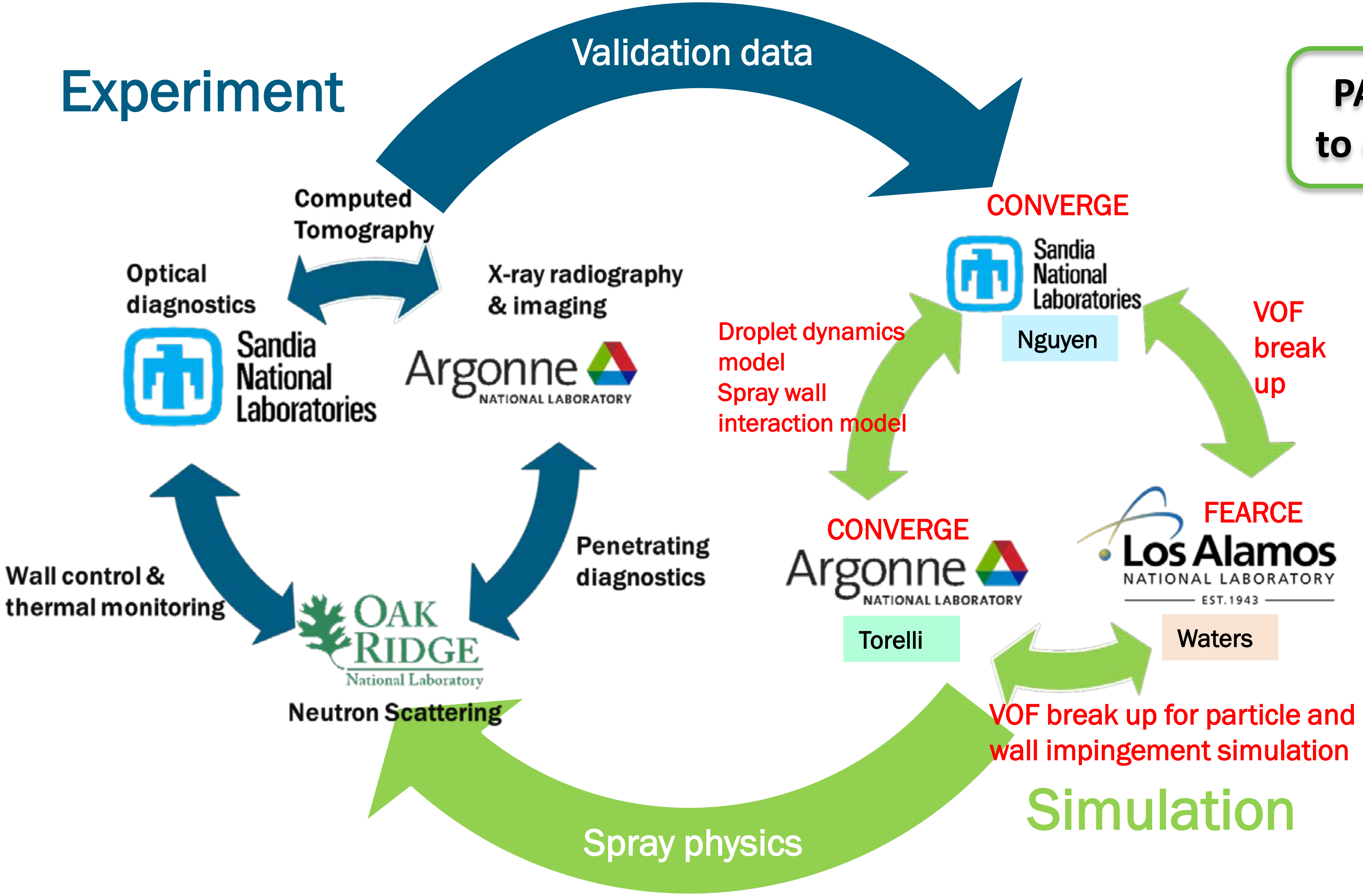
Overall Experimental Approach



- **Focusing on gasoline free spray phenomena**
- **Free sprays must remain a focus to**
  - Avoid wall impingement if possible
  - Have proper understanding of spray at time of wall impact
- **Coordinated experimental design**
- **Complementary diagnostics**
- **Deliver detailed validation data for CFD simulations**

Overall modeling approach, tied to experiments



PACE Sprays Team meets monthly to coordinate over 60 current tasks:

- **Focusing on gasoline free spray and impingement phenomena**
- **Simulations at target conditions with different modeling assumptions, compared to unique validation data**
- **Identify key weaknesses in spray and film models and take action to fix these weaknesses**

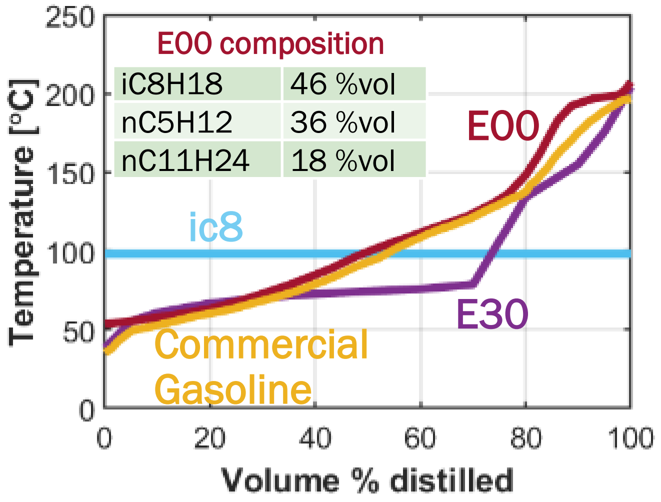
Free-spray target conditions: chosen for joint PACE research to "lay" the foundation for wall-film research at similar conditions

Operating conditions of interest for GDI applications

	T_{amb} [K]	P_{amb} [kPa-a]	ρ_{amb} [kg/m³]	T_f [K]	p_{inj} [MPa]	$T_{inj,hyd}$ [ms]	m_{inj} [mg]
G1	573	600	3.5	363	20	0.780	10
G2	333	50	0.5	363	20	0.780	10
G3	333	100	1.01	363	20	0.780	10
G2-cold	293	50	0.57	293	20	0.780	10
G3-cold	293	100	1.15	293	20	0.780	10
G3-double	333	100	1.01	363	20	0.462 0.900 dwell 0.327	6 + 4
G1-E00	573	600	3.5	363	20	0.780	10
G2-E00	333	50	0.5	363	20	0.780	10
G3-E00	333	100	1.01	363	20	0.780	10
G2-cold-E00	293	50	0.57	293	20	0.780	10
G3-cold-E00	293	100	1.15	293	20	0.780	10

Overview

- **Injector: ECN Spray G, 8-hole unit provided by Delphi**
- **Fuel: iso-octane/E00 three-component fuel**
- **Ambient: 100% N2**
- **Multi-component fuel is needed to match gasoline**
- **Using fuel proposed by Cordier et al. IJER 2019 with preferential evaporation measurements available**



<u>Importance of operating conditions</u> (many are ECN conditions)

G1: injection late during compression

- **knock control, lean dilute combustion, cold start**

G2: intake injection commonly encountered

- **flash-boiling; modeling weaknesses demonstrated**

G3: intake injection at 1 bar

- **standard patternator and other SAE J2715 data available**

double injection and cold fuel are applicable to cold start

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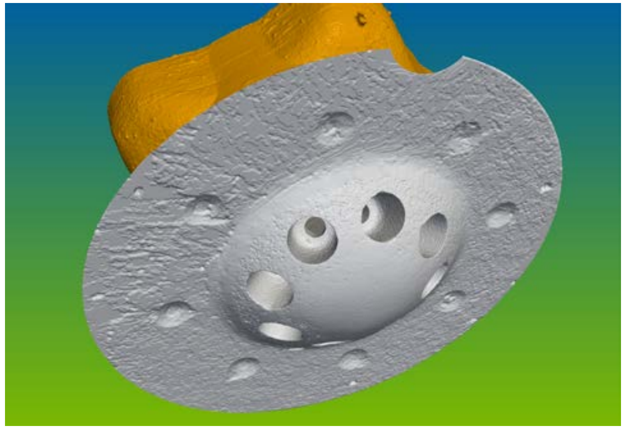
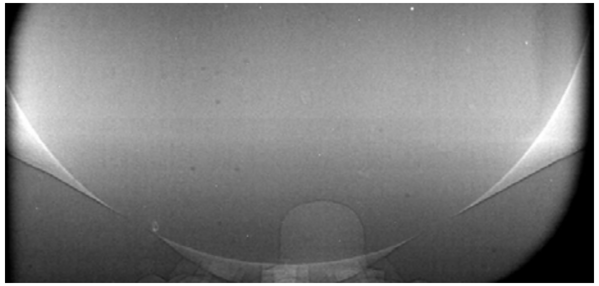
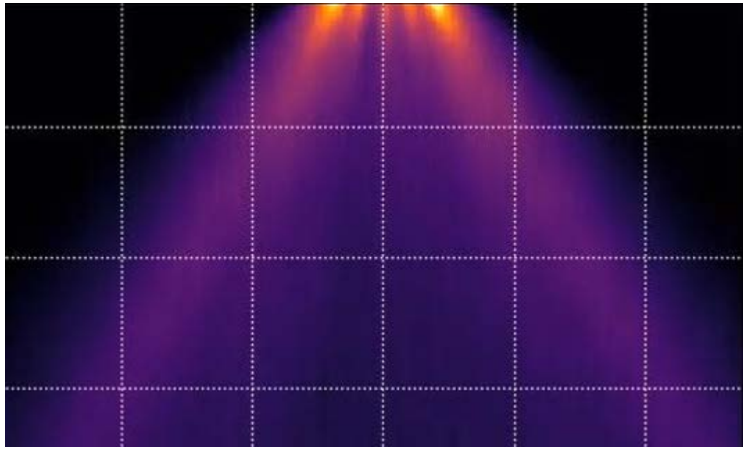
Approach
D.01.01: Free Spray and Wall Film X-ray Experiments (Powell)

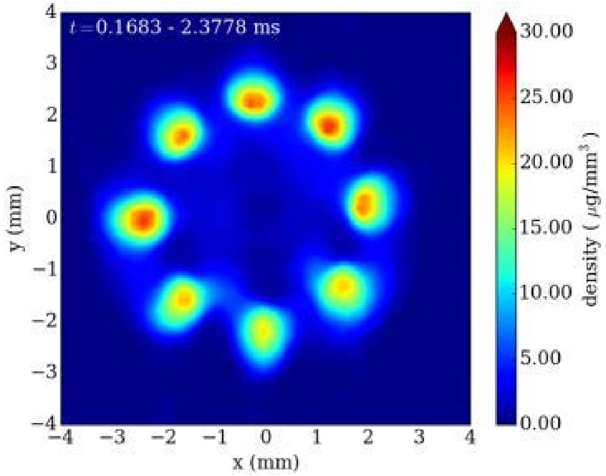
X-rays enable unique diagnostics for GDI fuel injection, both inside and outside the nozzle

- **Nozzle geometry:** Highest available spatial resolution for metrology, CFD mesh generation
- **Valve motion imaging:** Captures the time-resolved internal geometry
- **Radiography:** Quantifies the line-of-sight fuel distribution
- **Tomography:** Average 3-D fuel distribution, time-resolved









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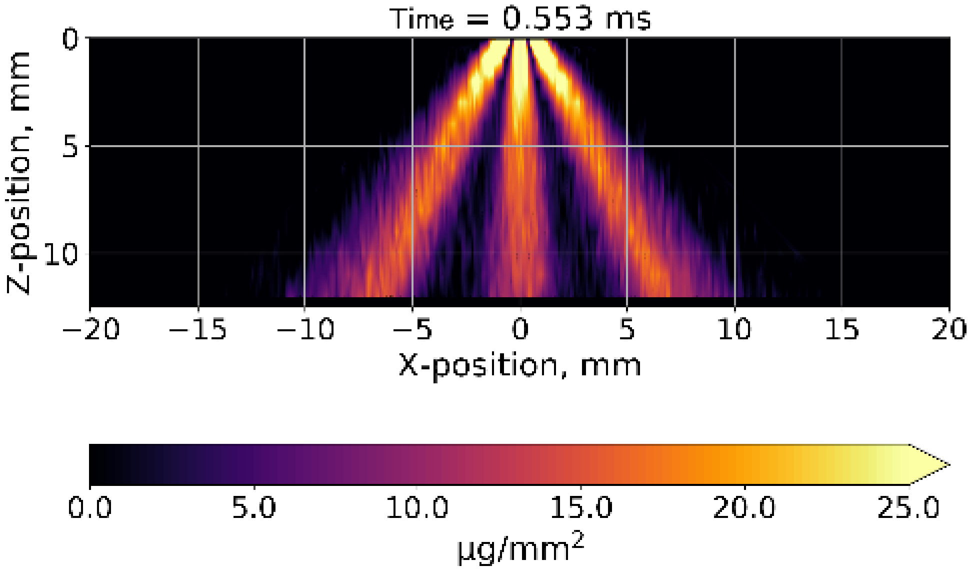
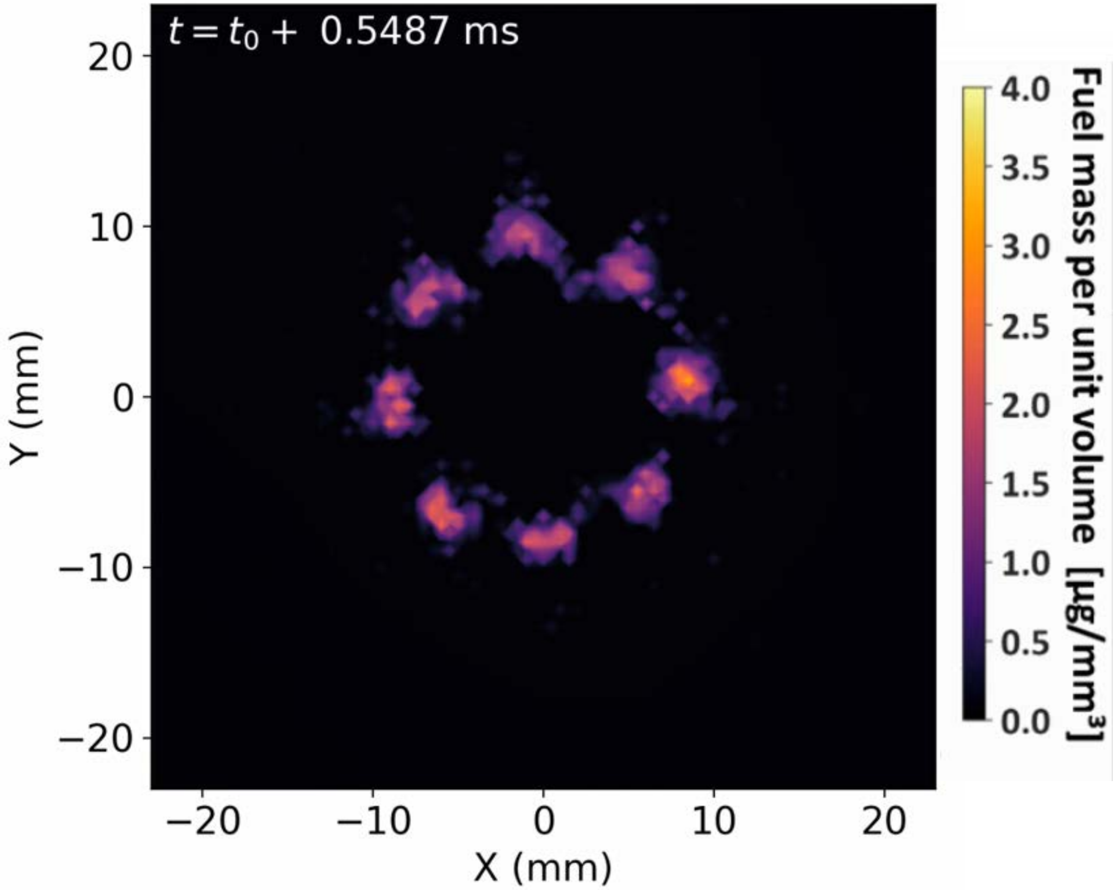
Technical Accomplishments and Progress
D.01.01: X-ray Tomography Measurements of Free Sprays (Powell)

- X-rays enable spray density measurements even in the near-nozzle region
- With multiple lines of sight, we can build up a 3D, time-resolved measurement of the average fuel density
- Results allow a quantitative comparison between measurements and simulation
- Much of this year's efforts were comparisons between free sprays and wall-impingement



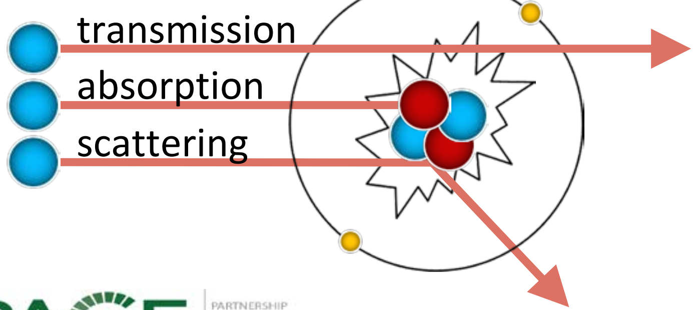


ECN Spray G3-cold, P_{inj}=200 bar, P_{amb}=1 bar, T=298K
Slice through spray at 12 mm

Approach
D.01.02: Neutron imaging of advanced combustion technologies (Wissink)

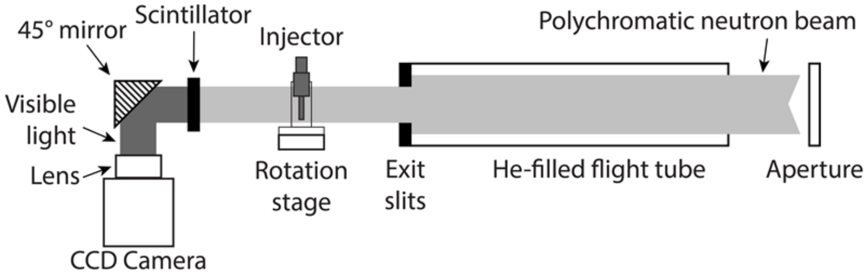
- Neutrons have the unique ability to easily penetrate most materials while also strongly interacting with certain isotopes like ^{1}H – <u>neutrons can see hydrocarbons through metal with high contrast</u>
- We are using cold neutron imaging at ORNL's High-Flux Isotope Reactor (HFIR) to investigate fuel injection and sprays in areas inaccessible to other diagnostics, providing a complementary approach to x-ray and optical experiments within PACE

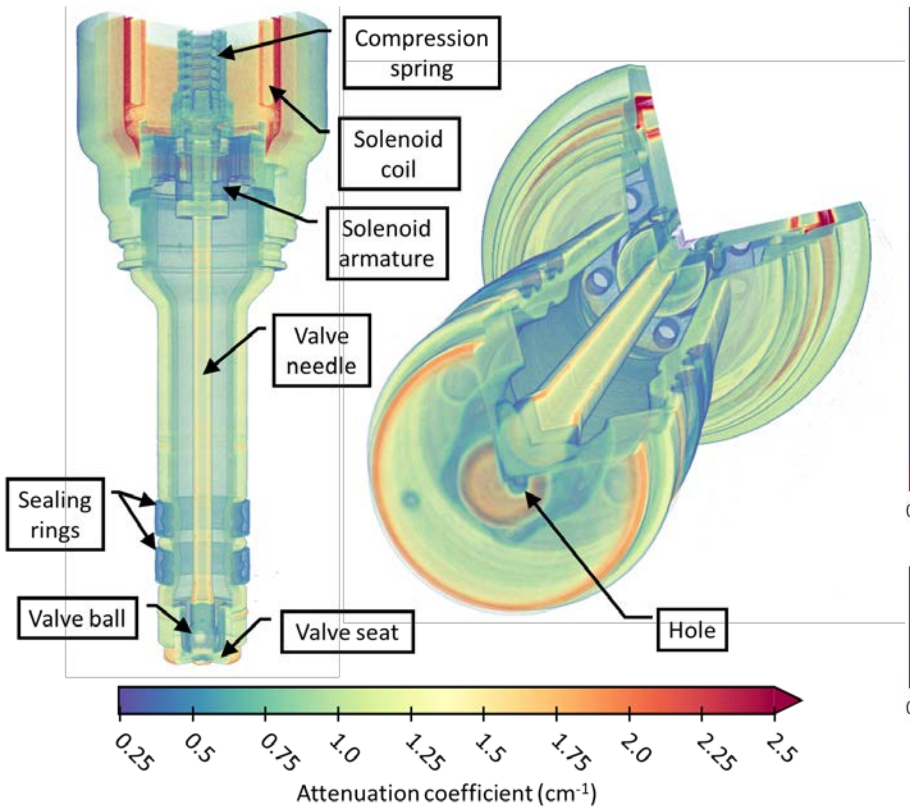
Neutrons



Neutron computed tomography

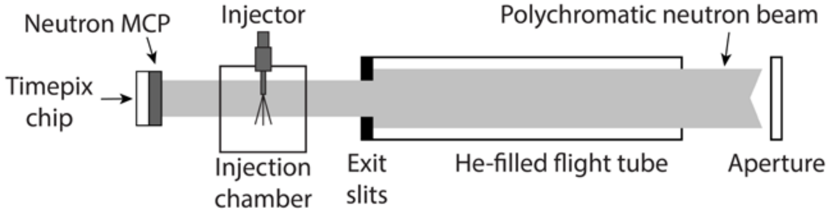
Detailed geometric information in thick metallic samples

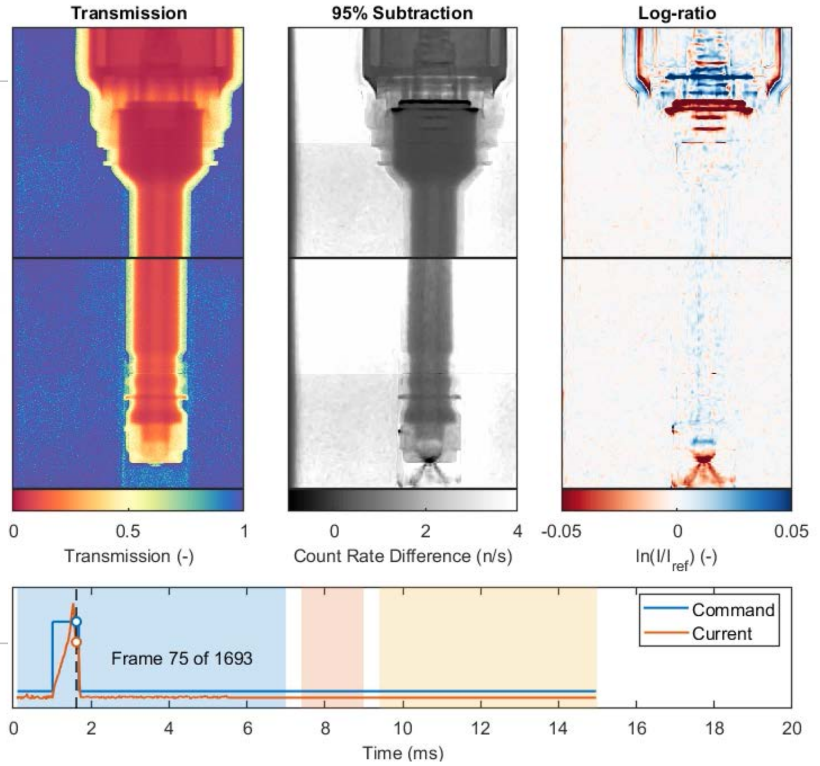




High speed neutron imaging

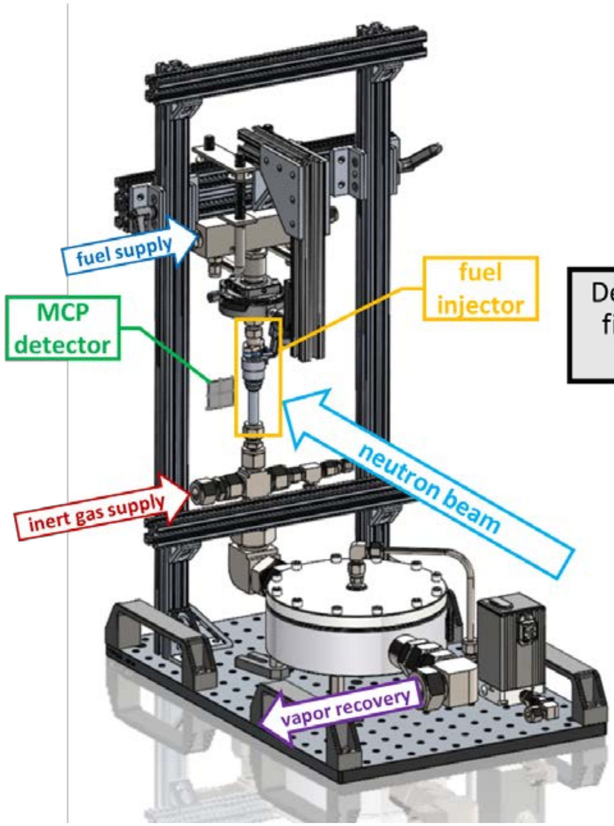
Mechanical and fluid dynamics inside metal devices

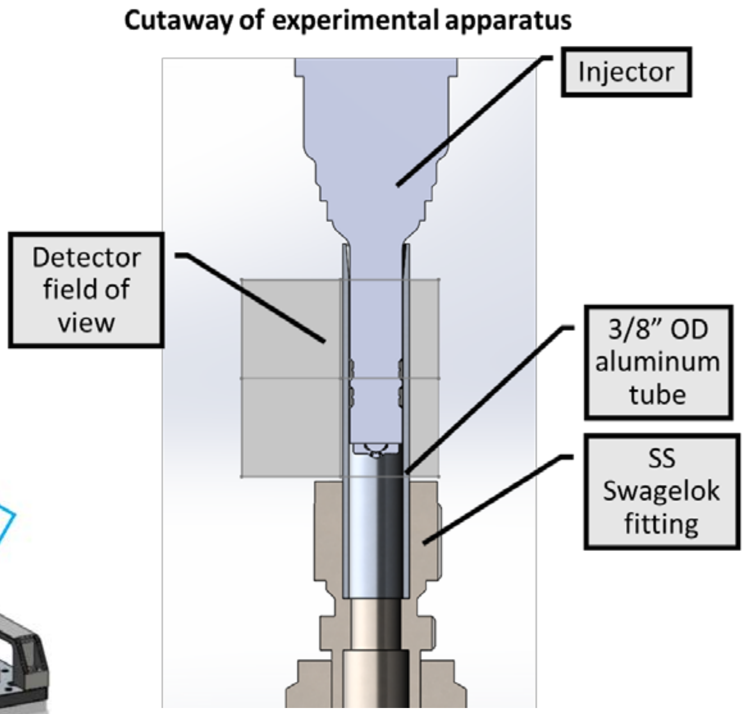


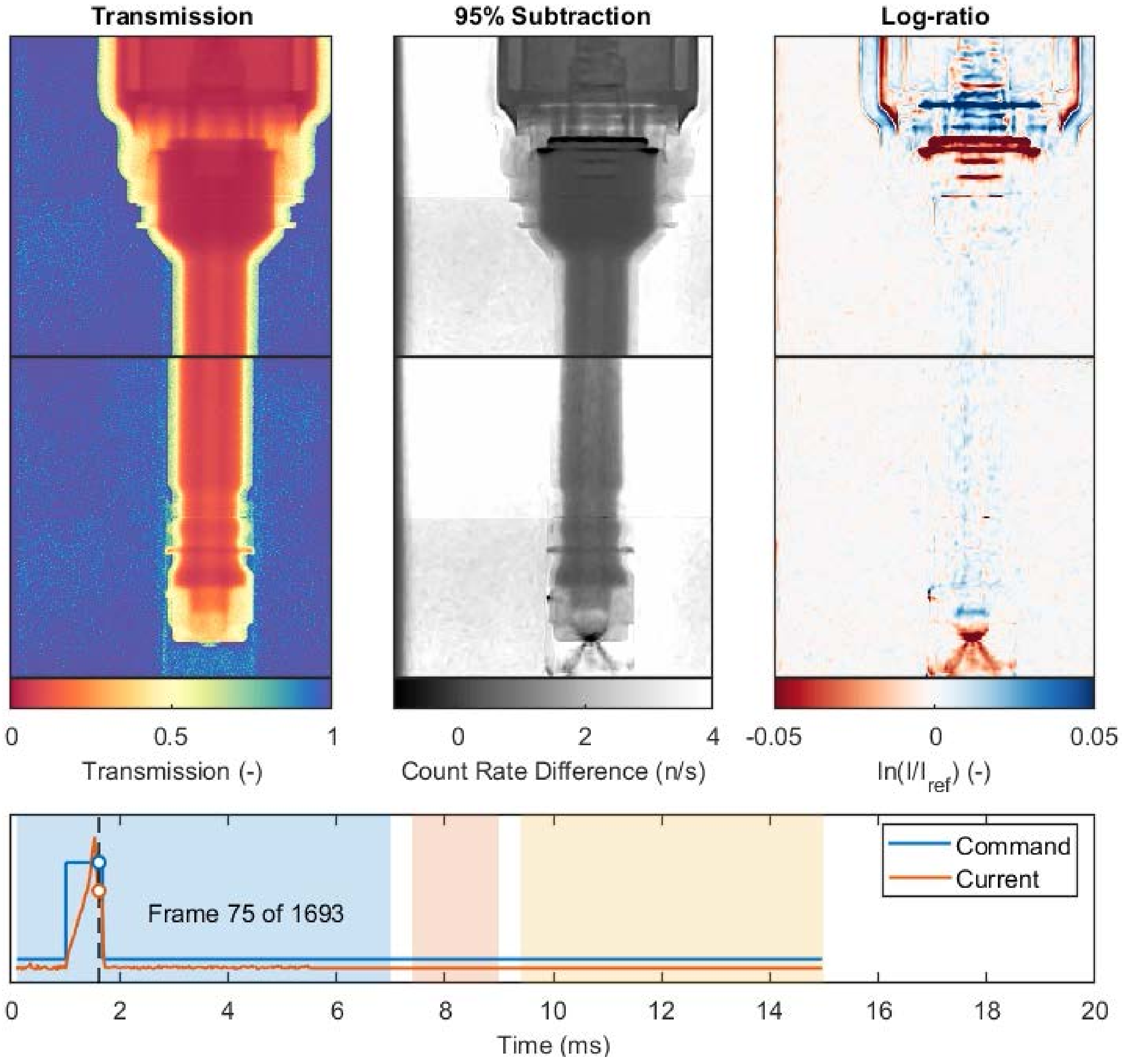


Technical Accomplishments and Progress
D.01.02: Neutron imaging of advanced combustion technologies (Wissink)

- **High-speed neutron imaging campaign in Nov 2019 captured the internal dynamics of a gasoline direct injector**







Technical Accomplishments and Progress
D.01.02: Neutron imaging of advanced combustion technologies (Wissink)

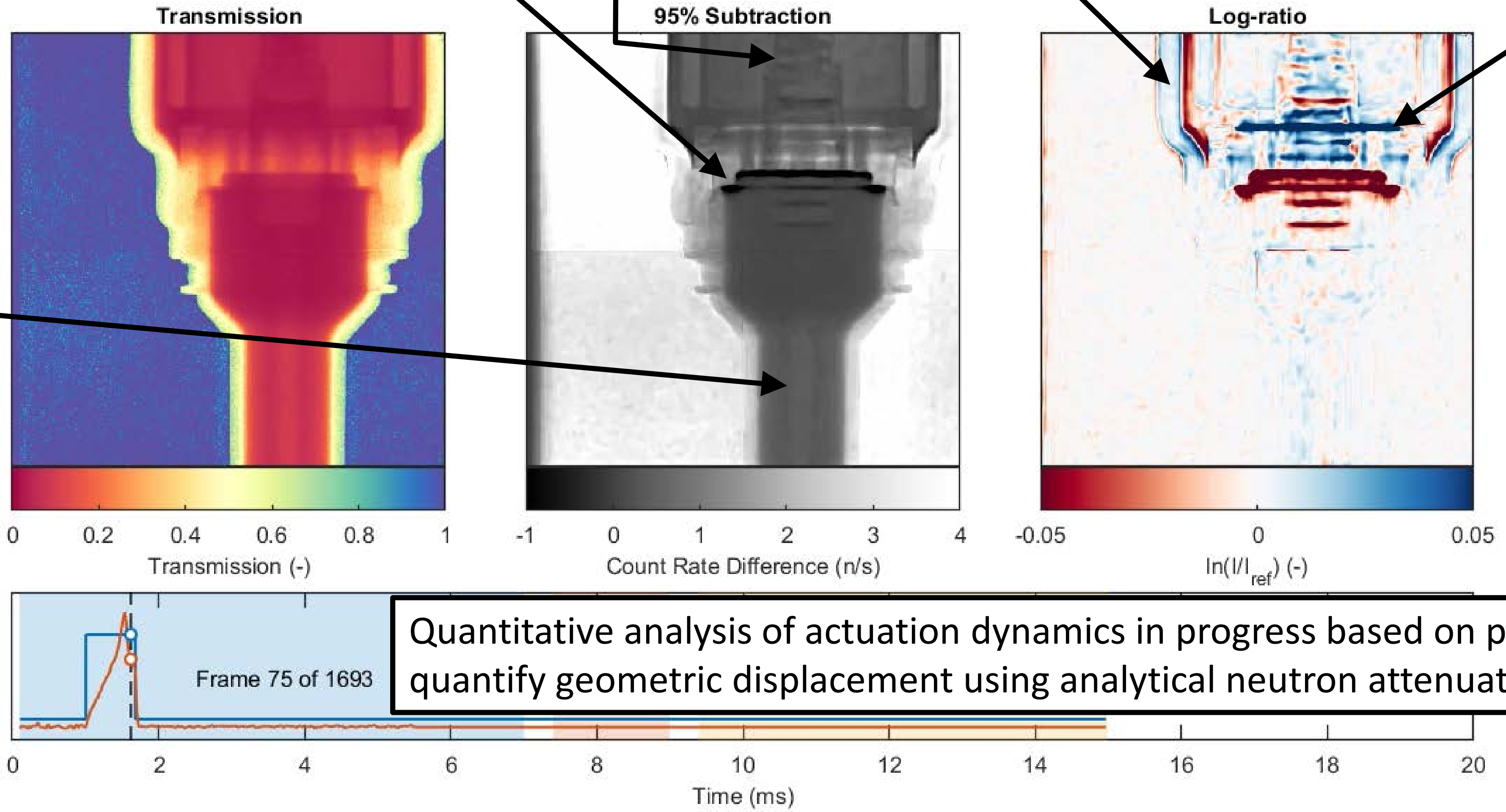
Armature bounces after injection and takes ~1 ms to settle – predicted by 1D models to be responsible for non-linear injection quantity (SAE 2014-01-1211)

Spring compression visible

Armature impacting the stop causes entire solenoid body to swell outward

Fuel must refill the gap between armature and stop – may have impact on settling time

Valve needle oscillates continuously during injection



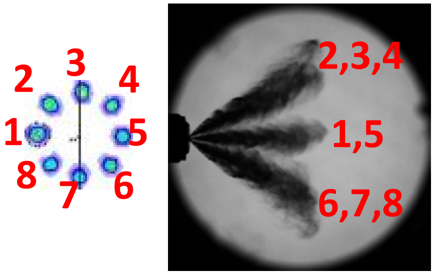
Quantitative analysis of actuation dynamics in progress based on previous work to quantify geometric displacement using analytical neutron attenuation model

Approach

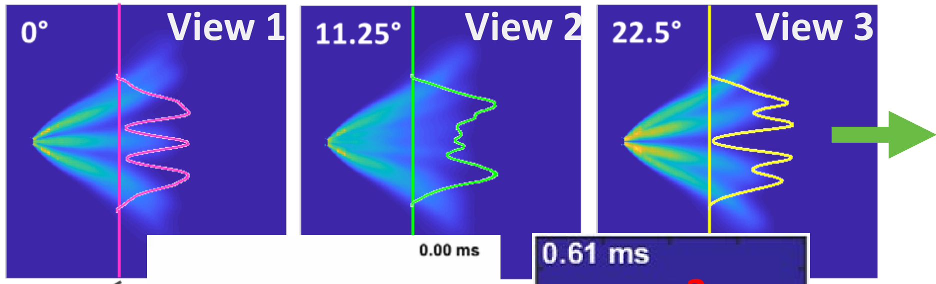
D.01.05: Free Spray and Wall Film Optical Experiments (Pickett)

- **Acquire liquid distribution using extinction imaging in large (125 mm window) chamber**
- **Convert to projected liquid volume using measured droplet size and setup extinction coefficient**
- **Use injector rotation and computed tomography to deliver 3D liquid volume fraction**
- **Uncertainties in LVF value are high in optically thick zones or because of droplet size assumption, but the technique accurately identifies plume position and liquid extent**

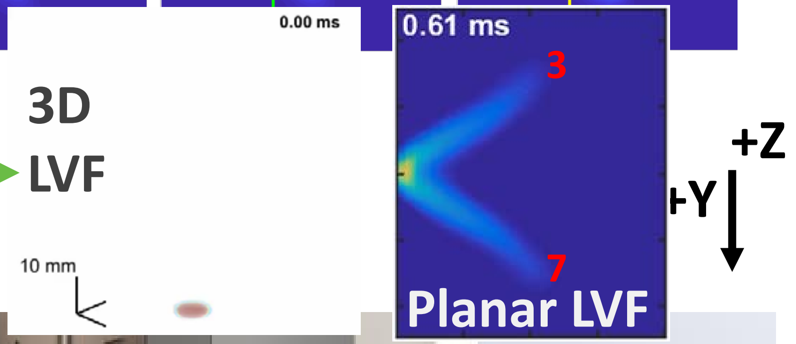
Raw data



Ensemble-average (300 injections)



Tomographic reconstruction

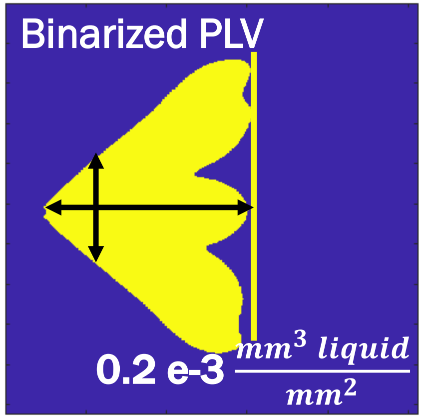


$$I/I_0 = e^{-\tau} \quad (1)$$

I: transmitted intensity

I_0: normalized baseline intensity

$$\tau = \int_{-y_\infty}^{y_\infty} C_{ext} \frac{LVF}{\pi d^3/6} dy \quad (2)$$



LVF: liquid volume fraction

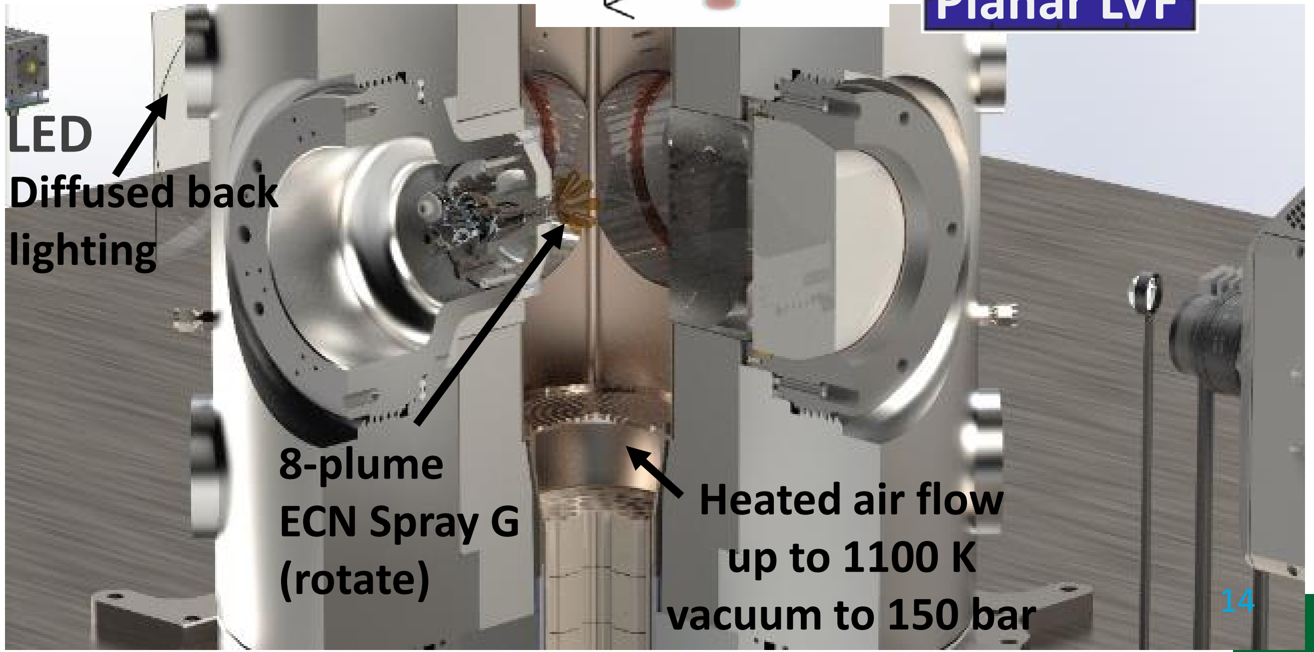
d: droplet diameter (7µm)

C_{ext}: extinction coefficient

τ: optical thickness

$$\tau \frac{\pi d^3/6}{C_{ext}} = \int_{-y_\infty}^{y_\infty} LVF \cdot dy \quad (3)$$

Projected Liquid volume: $\frac{mm^3\ liquid}{mm^2}$



- Droplet diameter was assumed as 7µm based on measurements from GM at G1 and SJTU at G2 conditions

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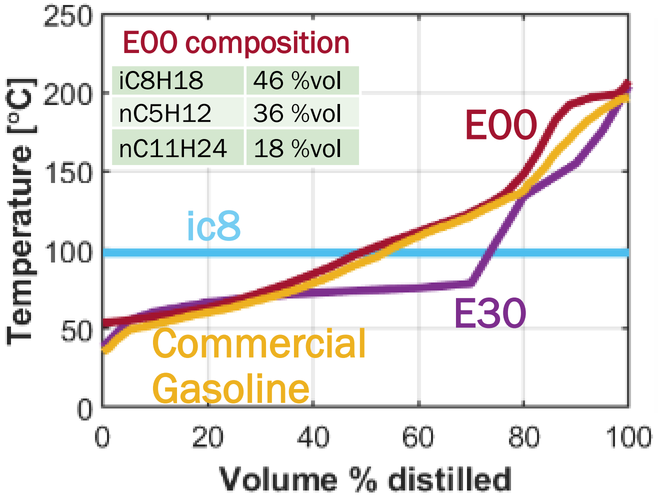
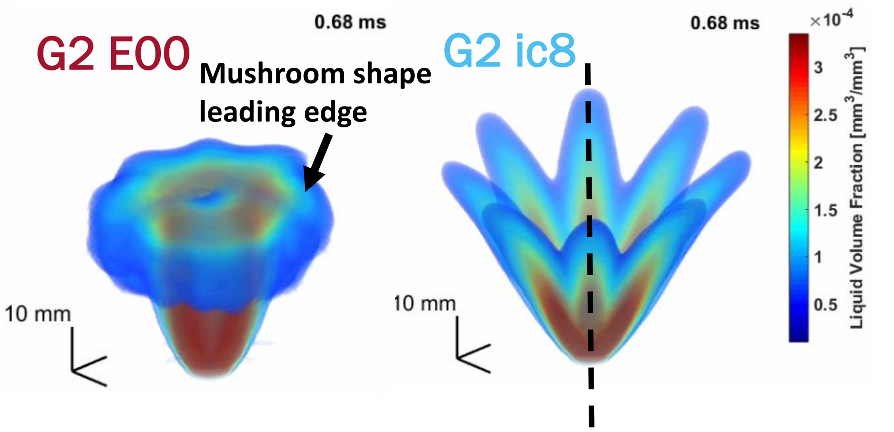
Technical Accomplishments and Progress
D.01.05: Measurements show liquid far past the usual in-cylinder wall position (Pickett)

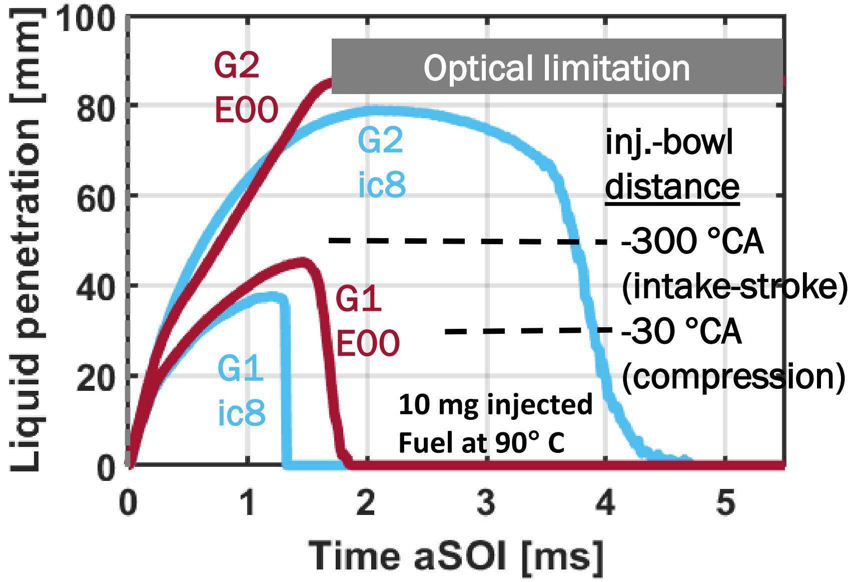
- **3-component surrogate (ECN E00) is representative of gasoline distillation curve**
- **Gasoline properties strongly affect spray behavior during intake injection (G2 condition)**
  - o Compare E00 to single-component iso-octane
  - o Plumes collapse to injector axis, ultimately reducing mixing with air and causing *greater* penetration
  - o High-BP fuels also cause longer liquid penetration
- **Wall wetting is a threat at both intake-injection conditions (G2) and compression-injection conditions. At G1 conditions:**
  - o Faster evaporation because of hot charge gas (573 K)
  - o Plumes do not collapse completely
- **Extinction imaging and computed tomography reconstruction provide valuable 3D dataset for CFD model validation**
  - o 3D dataset available online at ECN website for 12 PACE free-spray target conditions
  - o Used for side-by-side comparisons at PACE workshop in Feb 2020 and also at ECN7 (online June 2020)





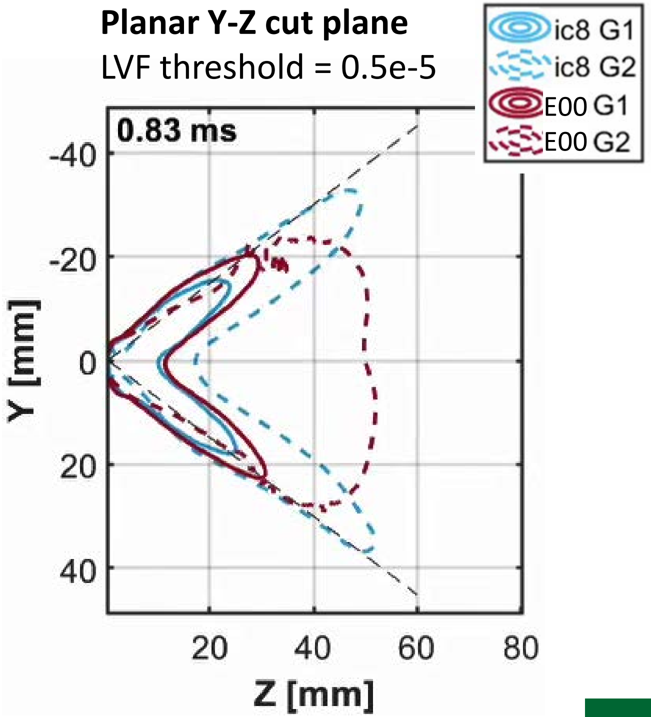
Line of sight extinction

projected liquid volume threshold = 0.2e-3 mm³ liquid/mm²



Planar Y-Z cut plane

LVF threshold = 0.5e-5



Sandia National Laboratories

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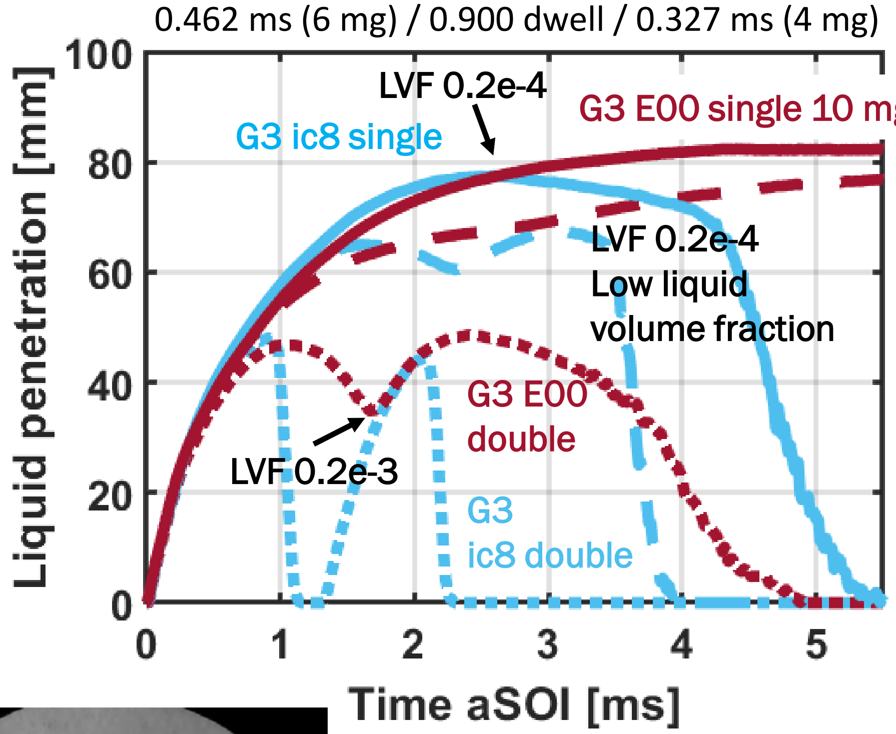
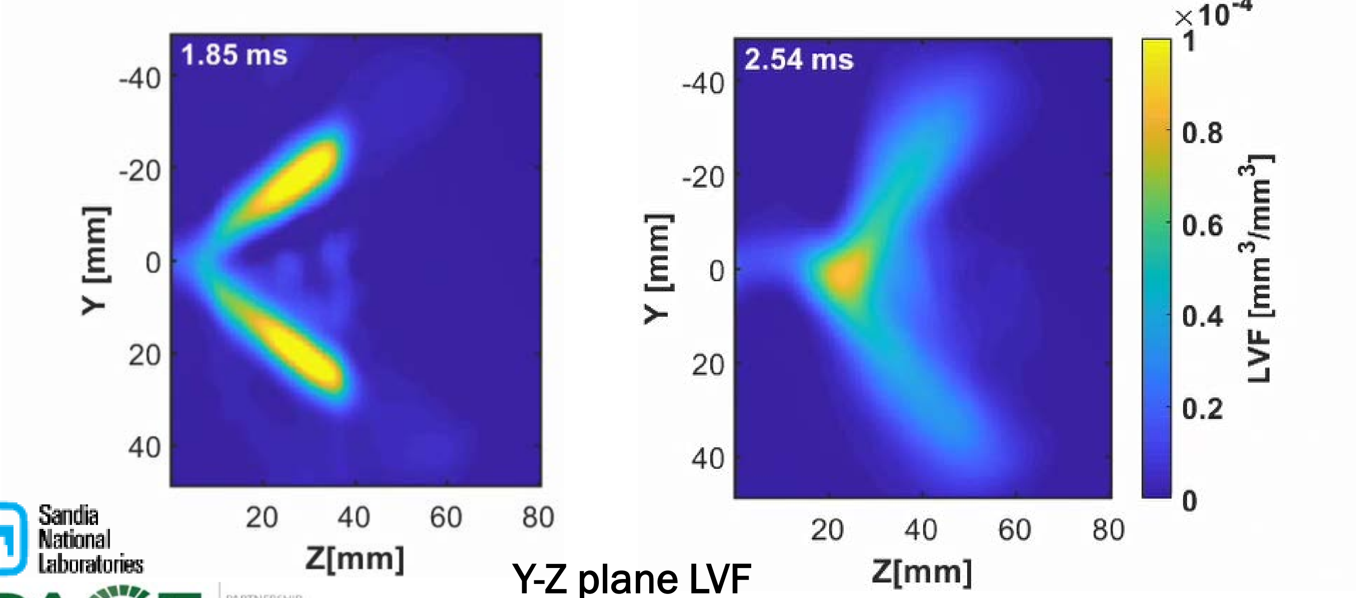
Technical Accomplishments and Progress
D.01.05: Multiple injections limit liquid penetration, could limit wall wetting (Pickett)

- **Split (or multiple) injections can limit liquid penetration**
  - Split injection (6 mg / 0.9 ms dwell / 4 mg) slows total jet penetration by 10 mm
  - But the LVF downstream of 50 mm (30 mm shorter) is significantly reduced (<0.2e-3)
  - Can also limit spray collapse as plumes maintain original trajectory
  - Split injection requires precise and capable injection hardware
- **Fuel effects remain important**
  - At G3 conditions, E00 penetrates longer because of slight collapse to jet center
  - A collapsed first injection (at G2 conditions) allows greater penetration for 2nd inject
  - and E00 vaporizes later because of its higher boiling boint components
  - Detail on these processes offered because of the 3D diagnostic

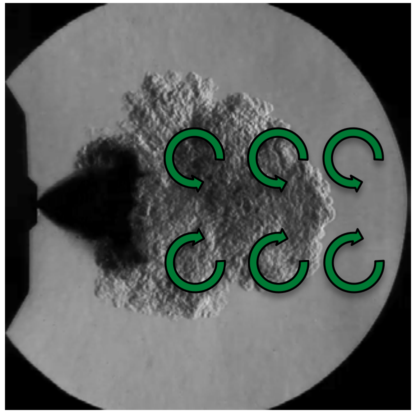


G3 double ic8

G3 double E00



Y-Z plane LVF



- E00 fuel shows much longer penetration length under G2 double-injection conditions.
- Liquid penetration moves forward following vortical motion from 1st injection.

G2 double E00 schlieren

Approach
D.01.03: Evaporative Spray and Soot Film Combustion Modeling (Nguyen)

- **Unified framework first proposed by Dahms and Oefelein (2016), herein called Corrected Distortion (CD) model**
  - Droplet distortion is modeled using the Taylor Analogy Breakup (TAB)
  - Viscous spherical drop coefficients are modeled using correlation from DNS data of Feng and Michaelides (2001)
  - Regression formulation of Richter and Nikrityuk (2012) provides non-sphericity correlation
- **Model implementation and validation via CONVERGE UDFs**

Standard model

$$C_d = C_{d,s}(1 + 2.632y)$$

$$C_{d,s} = \frac{24}{Re}\left(1 + \frac{1}{6}Re^{\left\{\frac{2}{3}\right\}}\right)$$

Particle equation of motion

$$\frac{dx_p}{dt} = u_p$$

$$\frac{du_p}{dt} = \frac{3}{4} C_d Re \frac{\mu}{(\rho_p d_p^2)}(u - u_p)$$

Particle equation of mass and heat transfer

$$\frac{dr_p}{dt} = \frac{\rho_g \mathcal{D}}{2\,\rho_l r_p} B_d Sh_p$$

$$\bar{A}Q_d = c_l m_p \frac{dT_p}{dt} - \frac{dm_p}{dt} H_{vap}$$

$$Q_d = \frac{Nu_p k_{air}(T_{air} - T_d)}{d_p}$$

Corrected Distortion model (2016)

$$C_d = C_{d,vis}\left(\frac{0.21 + \frac{20}{Re}\left(\frac{l}{d_p}\right)^{0.58} + \frac{6.9}{\sqrt{Re}}\left(\frac{l}{d_p}\right)^{-1.4}}{0.21 + \frac{20}{Re} + \frac{6.9}{\sqrt{Re}}}\right)$$

$$l = 2\,r_p(1 - C_b y)$$

$$C_{d,vis} = \frac{2-\lambda}{2} C_{d,b} + \frac{4\lambda}{6+\lambda} C_{d,2} \quad (0 \le \lambda \le 2;\ 5 < Re < 1000)$$

$$C_{d,vis} = \frac{4}{\lambda + 2} C_{d,2} + \frac{\lambda - 2}{\lambda + 2} C_{d,s} \quad (2 \le \lambda \le \infty;\ 5 < Re < 1000)$$

$$C_{d,b} = \frac{48}{Re}\left(1 + \frac{2.21}{\sqrt{Re}} - \frac{2.14}{Re}\right)$$

$$C_{d,2} = 17 Re^{-\frac{2}{3}}$$

$$C_{d,s} = \frac{24}{Re}\left(1 + \frac{1}{6}Re^{\left\{\frac{2}{3}\right\}}\right)$$

$$\lambda = \frac{\mu_l}{\mu_g}$$

- **Flash boiling model**
  - Based on experimental results of Adachi et al. (1997)
  - Calculate superheated vapor generation due to flash boiling phenomenon
  - Treat the Eulerian pressure as droplet pressure

$$\frac{dM}{dt} = \frac{\alpha\,\Delta T\,A_p}{h_{fg}}$$

$$\alpha = 760\,(\Delta T)^{0.26} \quad (0 < \Delta T < 5)$$

$$\alpha = 27\,(\Delta T)^{2.33} \quad (5 < \Delta T < 25)$$

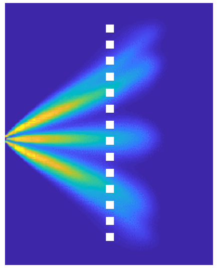
$$\alpha = 13.8\,(\Delta T)^{0.39} \quad (\Delta T > 25)$$

$$\Delta T = T_p - T_{boil}$$

- **Preferential evaporation approach**
  - Using available discrete multi-component model within CONVERGE to treat evaporation
  - Individual species evaporate according to Raoult's ideal mixing rules—requires thermo properties for each component

Technical Accomplishments and Progress
D.01.03, D.01.05 : New method to assess wall-wetting potential (Nguyen, Pickett)

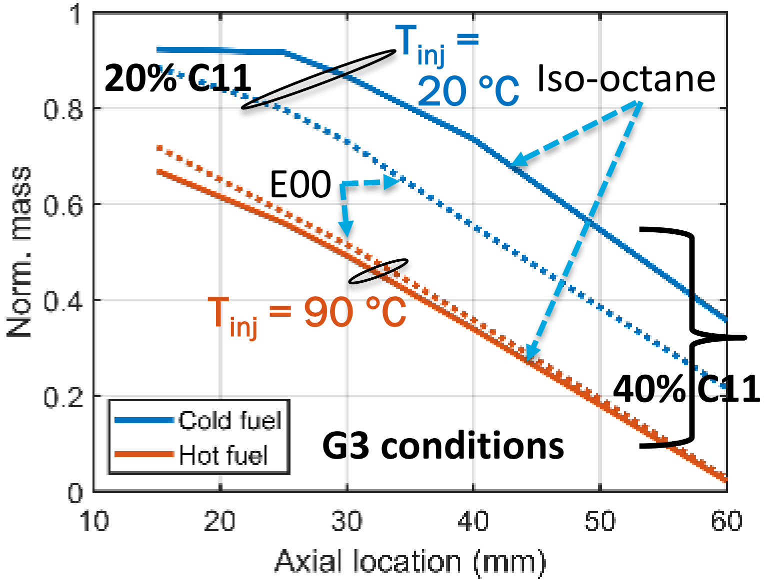
Method: Develop tool to assess potential for wall wetting, using free-spray simulations



$mass_{inject}$ = 10 mg

$$norm_{mass}\Big|_{z=z_a} = \frac{\overbrace{\iint \rho_p(x,y)U_p(x,y)\,|_{z=z\_a}\,dA\,dt}^{\textbf{Mass flow rate of liquid at specific axial plane}}}{mass_{inject}}$$

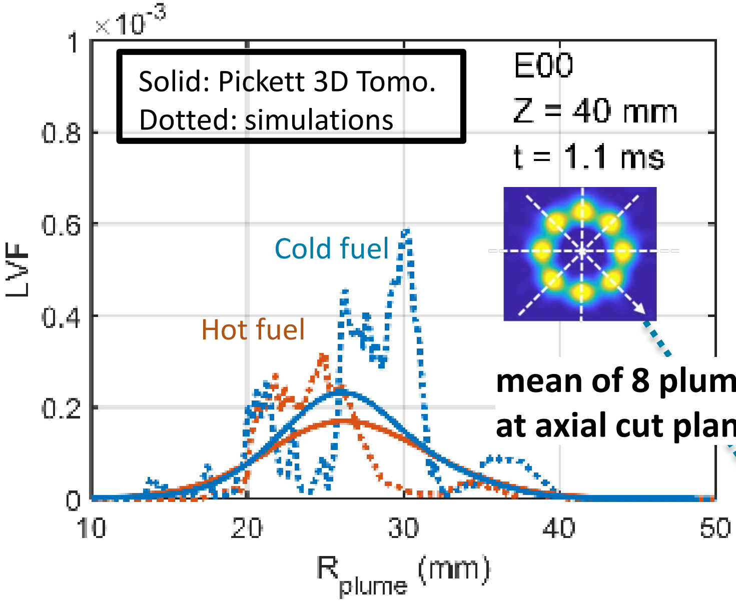
Predicted mass crossing wall plane for 2 fuels & 2 fuel Temp's

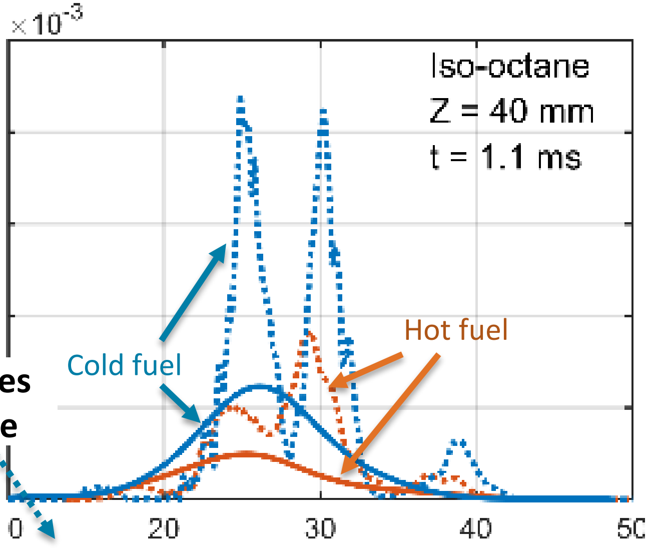


Remaining fuel becomes progressively heavy (C11), and with higher surface tension to adhere to wall ($\sigma_{C11} \approx 2 \cdot \sigma_{C5}$)

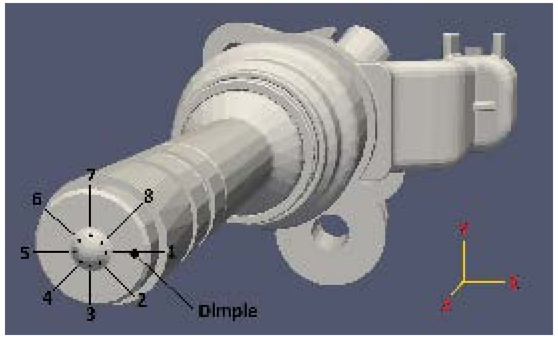
Substantial potential for wall wetting predicted, even with relatively small injected mass (10 mg)

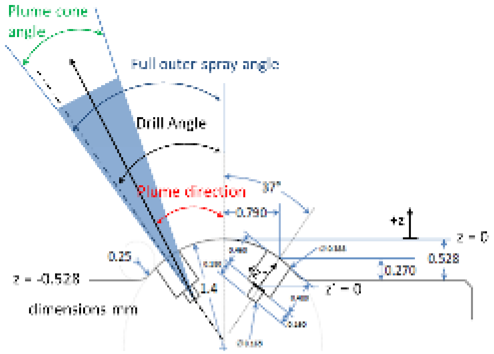
- **Compare against experimental LVF measurements to gain confidence in predictions, understanding that LVF is not the same as normalized mass (a flux term)**
- **Trends are confirumed, though higher LVF is predicted despite enhanced evaporation (corrected distortion) model**
- **When cold, E00 has lower LVF than iso-octane, when hot, E00 has higher LVF. Fractional distillation of E00**
- **In reality, liquid fuel impinging on the wall will be less than the predicted normalized mass, but this establishes a method assessing wetting potential with multi-component fuels**





Approach
D.02.01: Free-Spray Simulations (Torelli)





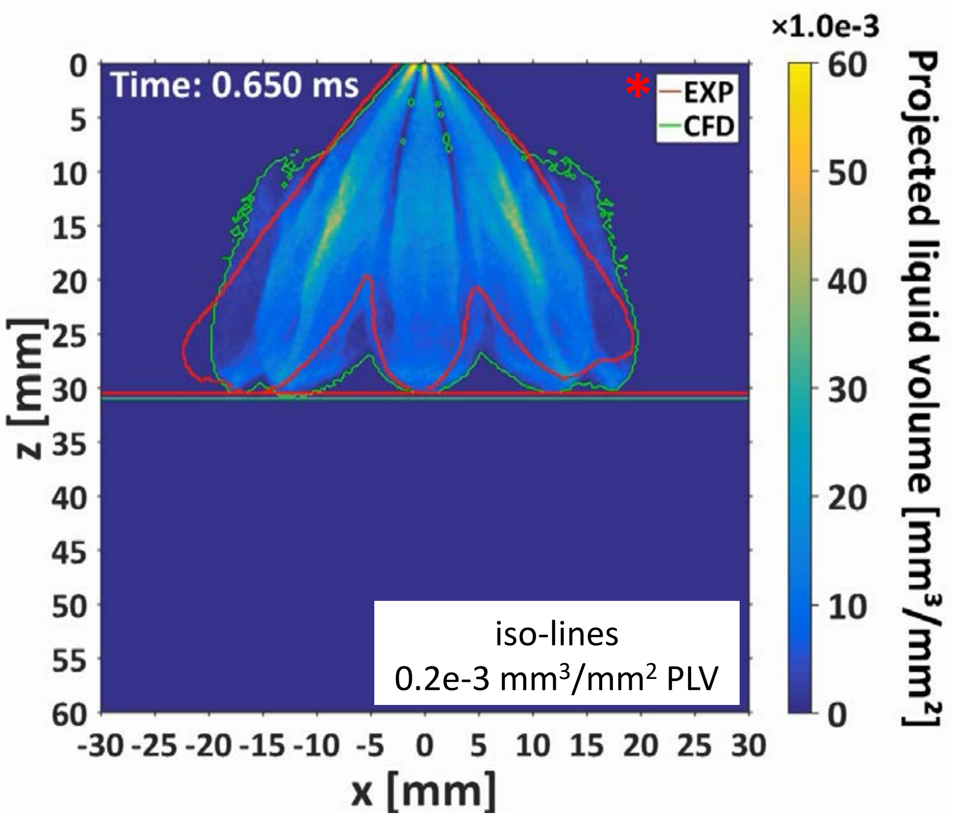
The Spray G injector was used for all the simulations:

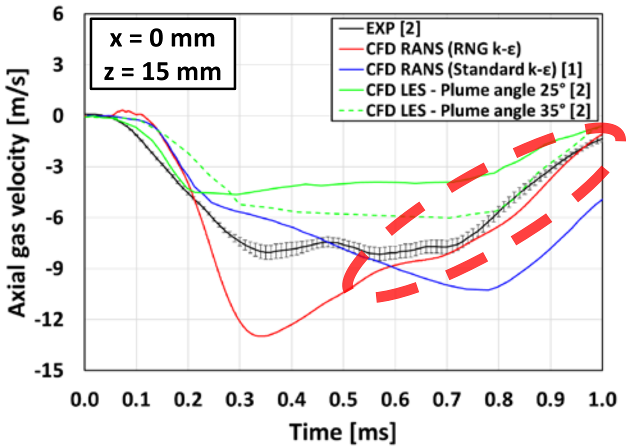
- A standardized reference system allowed for consistent comparisons between experimental and numerical datasets, as well as among different institutions;
- Exact computational domain was modeled after the X-ray chamber (rather than the typical box/cylinder)

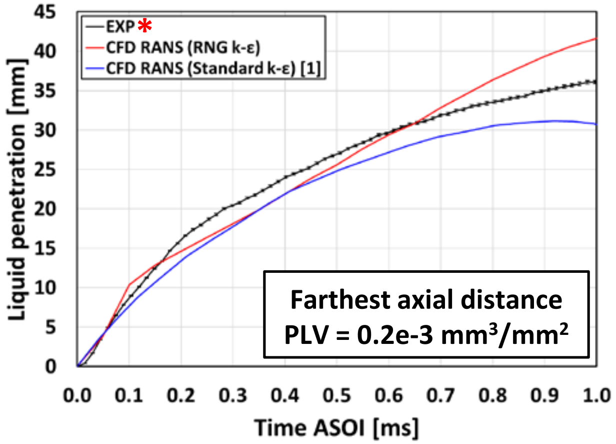
- All existing setups were ported to CONVERGE v3.0 leveraging previous RANS and LES work from Argonne;
- Improved prediction of GDI free-spray behavior are key to ensuring the correct boundary conditions for spray-wall interaction models (**Torelli et al, IJER, 2020**);
- **Standard k-eps is not the preferred model for engine simulations, hence the initial effort focused on RNG k-eps**;
- New, dedicated post-processing tools that can read directly from CONVERGE's output were developed for consistent quantitative comparison against X-ray experiments
- Post-processing tools and new models can be made available to industry.

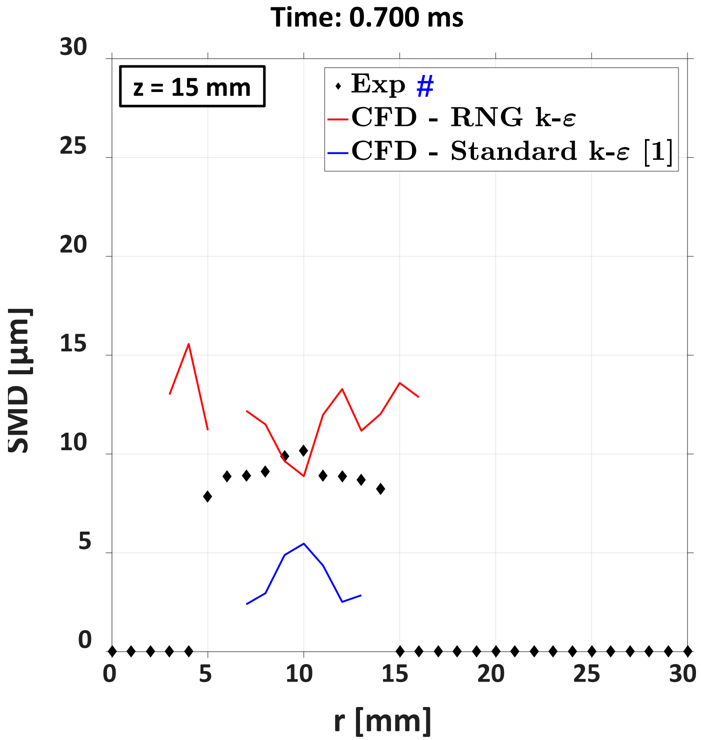
Technical Accomplishments and Progress
D.02.01: Global and Local Characterization of Free Sprays (Torelli)

- Iso-octane fuel under G1 condition (T=573 K, p=600 kPa)
- Sandia's experimental measurements of initial turbulence and 3-D tomography of liquid volume fraction* were respectively used to initialize the flow field and impose spray cone angle vs. time and average plume angle as boundary conditions
- The combination of a new spray setup and RNG *k-ε* turb. model led to improved droplet sizes and axial gas velocity predictions
- Some differences still remain to be addressed, but we believe these results are sufficient to address spray wall interaction









[1] Nocivelli et al., SAE Tech. Paper, 2020-01-0330, 2020

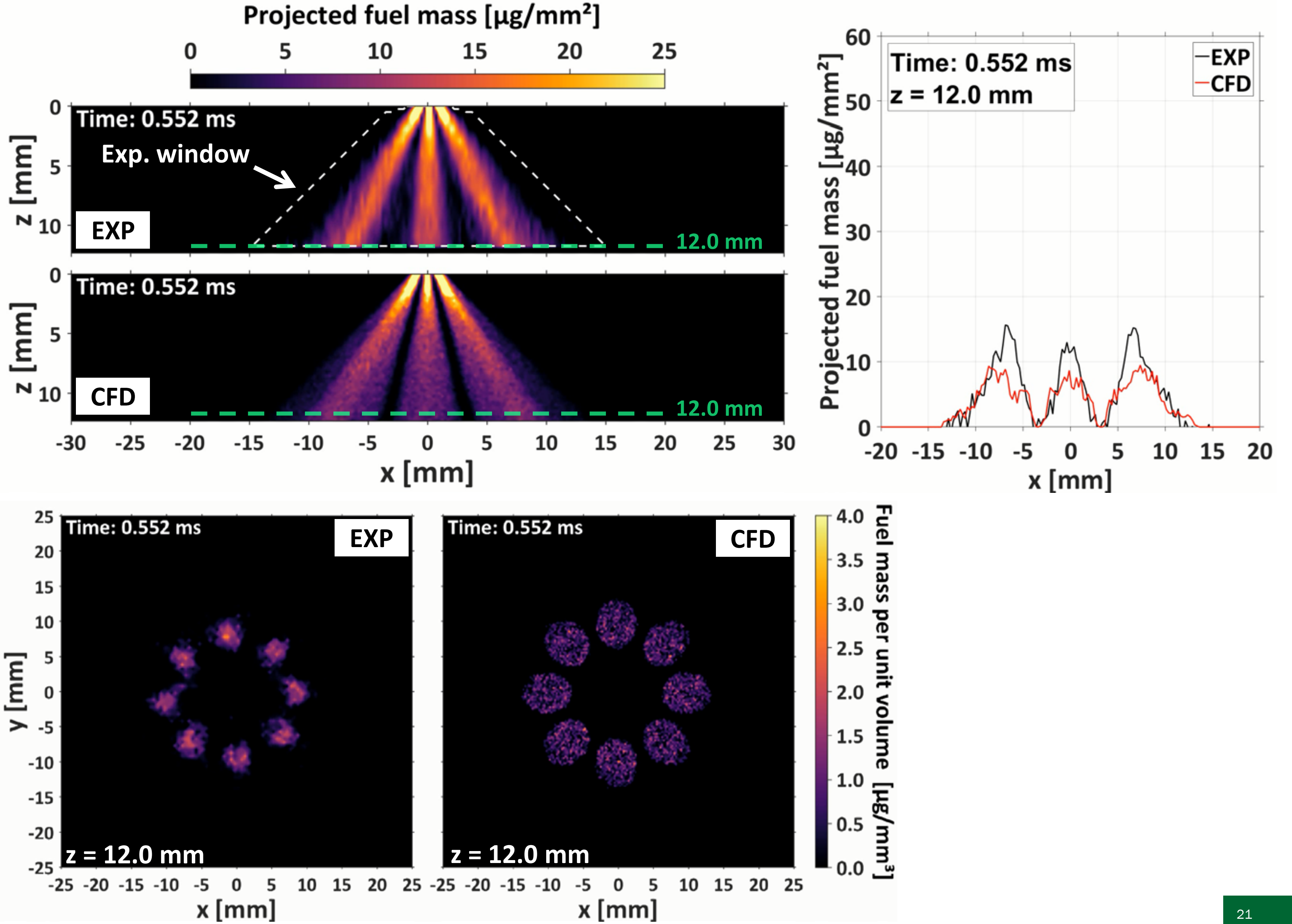
[2] Sphicas et al., SAE Int. J. Fuels & Lubr. 2017-01-0837, 2017

* Hwang and Pickett, Sandia National Laboratories

\# Parrish, General Motors

Technical Accomplishments and Progress
D.02.01: Global and Local Characterization of Free Sprays (Torelli, Powell)

- Exact same G1 setup condition applied to G2, G2-cold, G3, and G3-cold cases
- Simulation of G3-cold case (T=298 K, p=100 kPa)
- Projected fuel mass showed excellent agreement in the first 5 mm downstream of the injector tip
- Good agreement found at other downstream locations, including at 12 mm, i.e., 0.3 mm away from the location of the impingement plate in the X-ray experiments of spray-wall interaction
- Good results were also achieved in terms of fuel mass per unit volume by comparison of CFD results and X-ray experimental data



PACE PARTNERSHIP TO ADVANCE COMBUSTION ENGINES

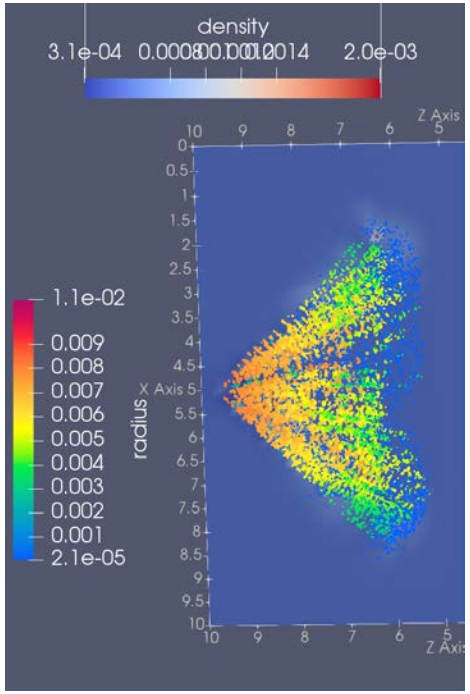
Approach
D.02.02: Free Spray and Wall Impingement, Including VOF (Waters)

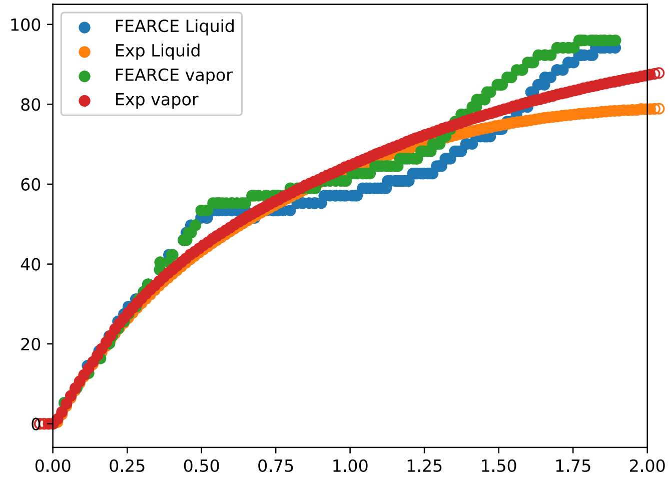
- FEM gas phase coupling with Lagrangian particle method (droplet phase)
  - Gas and droplet velocity: superscript ‘*n*’ current time, subscript ‘*n*’ nodal gas, e.g. ρ_n^n modal density current time. Solving for $U_n^B\ and\ V_P^B$
  - Droplet velocity: $\frac{V_p^B - V_p'}{\Delta t} = D_p(U_n^B + U_p' - V_p^B)$ (1)
    - where $D_p = \frac{\rho_n^n}{\rho_d} \frac{|U_n^n + U_p' - V_p'|}{r_p^A} C_D(Re_p)$
  - Gas velocity: $M'^B_n U_n^B - M'^n_n U_n^n = E_n - \sum N_p' \frac{4}{3}\pi\rho_d[(r_p^B)^3 V_P^B - (r')^3 V_p']$ (2)
    - V_p^B droplet velocity, V_p' at n particle velocity, U_p' gas turbulence adds, U_n^B gas velocity and E_n contributions to the Lagrangian phase momentum except those due to spray momentum exchange.
- Equation (1) and (2) are solved together implicitly => circumventing ‘dt’ limitations strong velocity phase coupling.
- Finite element system for droplet motion,
  - Two-way coupling and stress analysis is grid convergent;
  - Uses 2nd order interpolation to evaluate sub-grid scale stresses, and property values.
  - Unique to FEM versus traditional CFD where the Lagrangian particle methods are not 2nd order accurate at a minimum
  - Traditional CFD not generally grid convergent, requiring higher resolution.
- KH-RT model for break-up.
  - KH primary and secondary break-up with blob model injection.
  - This modified KH, determines the surface area amenable to droplet fracture/separation, being the trough of unsteady surface waves.
  - The RT model is generally being employed as secondary break-up.
- Spherical droplet assumption with internal heat transfer for early modeling of surface T and partial pressures.
  - Sub-grid scale evaluated by 2nd order interpolation => grid convergence

Technical Accomplishments and Progress
D.02.02: FEARCE Simulations at ECN G2 Conditions (Waters)

G2(T=333, P=50kPa)

- Secondary break up by RT is important for the G2 case
- With only primary breakup, G2 ends up with too many particles
- Collision is on for all cases.
- For G2 (flash boiling), energy transfer is barely considered between flash evaporated particles and gas background.
- Plots show that G2 is a significantly wider than G1.





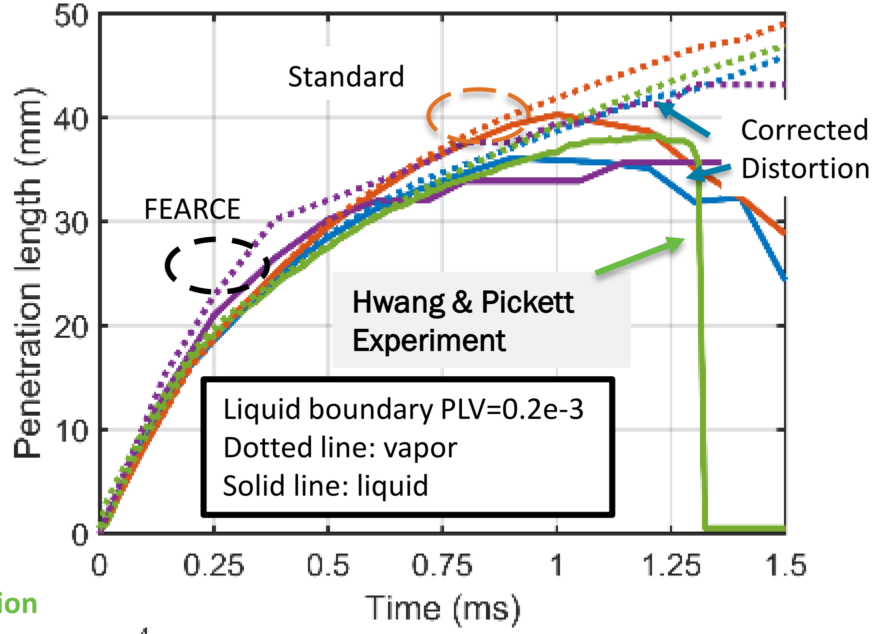
Both liquid and vapor tend to overshoot.

Particle (radius of particle in rainbow) and vapor (red and blue) at t=6.8e-4 s.
The spray lost its symmetry later in time.

Technical Accomplishments and Progress
D.01.03, D.02.01, D.02.04 : Predictions of Penetration, LVF (Nguyen, Torelli, Waters)

- **CONVERGE 2.4 simulation (SNL)**
  - Due to enhanced evaporation of highly distorted drops, Corrected Distortion (CD) model predicts lower Liquid Volume Fraction (LVF)
  - Still over-predicts experimental data after the end of injection (t > 0.78 ms)
  - CD model captures plume movement toward the injector axis (R_plume = 0), similar to experimental observation

- **CONVERGE 3.0 simulation (Argonne)**
  - Larger LVF than experiments but SMDs (shown later) consistent with GM (Parrish) experiments at Z = 15 mm
  - Larger plume width
  - Plume movement towards centerline after end of injection

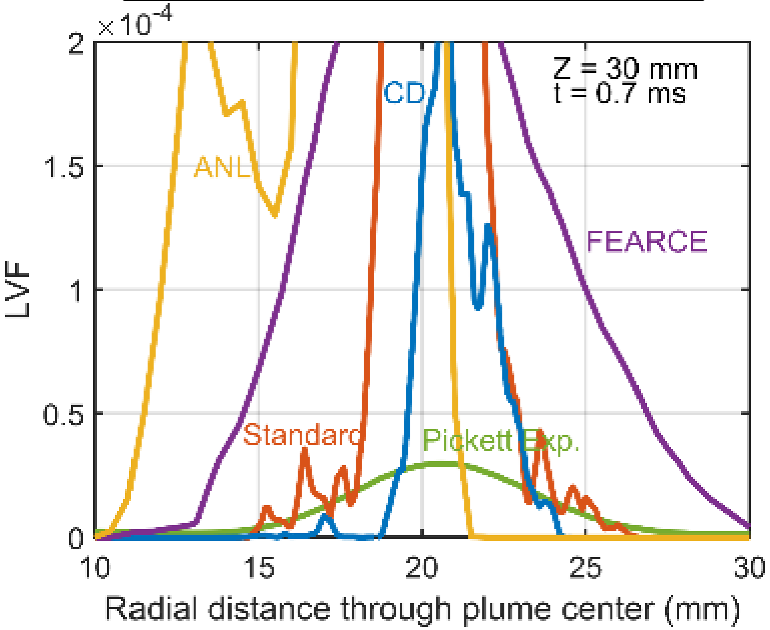


CD: Corrected Distortion
Standard: Frossling +Dynamic Drag

- **FEARCE simulation (LANL)**
  - Investigating resolution and other grid dependencies
  - Signs of insufficient evaporation leading to higher liquid volume fraction
  - Also investigating G2 and G3 conditions

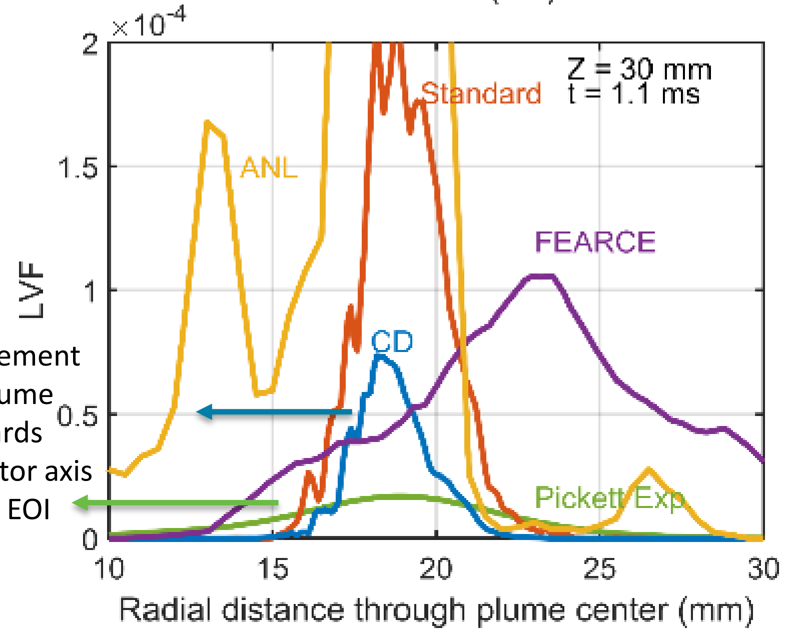
G1 Ambient Condition

T=573 K, P=600 kPa



End of injection

Movement of plume towards injector axis after EOI



Collaboration and Coordination with Other Institutions

- Collaboration within the sprays team and across PACE
- Collaboration with the Engine Combustion Network on target conditions
- 15 Industry partners in the AEC MOU for direction and feedback

Task	Description
D.01.01 Powell	• Internal collaboration with Argonne X-ray Sciences Division • Lead for ECN GDI Internal Flow studies
D.01.02 Wissink	• Injector hardware provided by GM, Delphi, Bosch • Internal collaboration with ORNL Neutron Sciences Directorate to develop new detector hardware and improve quantitative data analysis techniques
D.01.03 Nguyen	• Partnership with Convergent Science Inc. for model implementation to make results available to the engine community
D.01.05 Pickett	• Engine Combustion Network Leadership
D.02.01 Torelli	• Collaboration with Michigan Tech and UMass-Dartmouth for spray-wall interaction modeling

Remaining Challenges and Barriers

- **PACE-wide barriers are discussed in ACE138**
- **Experiments**
  - Experiments are testing relatively old hardware. There is a task to reevaluate this next year
  - Limited data on shot-to-shot variability
  - Limited data on the effects of gas flows
- **Simulations**
  - Uncertainty in plume cone and plume direction angles. This needs to become predictive
  - Sensitivity to initial turbulence level and its influence in fuel jet spreading rate
  - Overpredicting liquid volume fraction, underpredicting vaporization
  - Multi-component fuels are still a challenge
  - The effects of gas flows are a challenge

Proposed Future Research

- **D.01.01: Free Spray and Wall-Film X-ray Experiments (Powell)**
  - Spray measurements with multi-component fuels
- **D.01.02: Neutron Imaging of Advanced Combustion Technologies (Wissink)**
  - High-speed imaging of solenoid armature dynamics with multiple close-coupled injections for boundary conditions and validation of electromagnetic/hydraulic models
- **D.01.03: Evaporative Spray and Soot Film Combustion Modeling (Nguyen)**
  - Modeling flash boiling conditions with preferential evaporation
- **D.01.05: Free Spray and Wall-Film Optical Experiments (Pickett)**
  - Increased throughput for variability studies
- **D.02.01: GDI Spray-Wall Interaction Modeling (Torelli)**
  - Multi-realization LES to evaluate injection-injection variability at spark using Sandia's SIDI platform
- **D.02.02: Free Spray and Wall Impingement, Including VOF (Waters)**
  - Investigate better evaporation, mass transfer, drag models for the free spray.

Any proposed future work is subject to change based on funding levels

Summary

- **D.01.01: Free Spray and Wall-Film X-ray Experiments (Powell)**
  - Near-nozzle spray measurements have been completed, used for model validation
- **D.01.02: Neutron Imaging of Advanced Combustion Technologies (Wissink)**
  - Experiments have visualized GDI armature bounce at end of injection, other actuation dynamics
  - Actuation dynamics will quantify displacement of injector needle using analytical attenuation model
- **D.01.03: Evaporative Spray and Soot Film Combustion Modeling (Nguyen)**
  - Fully-coupled Corrected Distortion with Adachi model has predictive potential for wall-wetting conditions
- **D.01.05: Free Spray and Wall-Film Optical Experiments (Pickett)**
  - Downstream LVF measurements have been completed, used for model validation
- **D.02.01: GDI Spray-Wall Interaction Modeling (Torelli)**
  - New spray setup coupled with RNG k-eps led to improved predictions of SMD, gas velocity, and fuel mass
- **D.02.02: Free Spray and Wall Impingement, Including VOF (Waters)**
  - Particle method combined with Finite element method tested and validated at GDI-relevant conditions

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Technical Backup Slides

Remaining Challenges and Barriers

- **D.01.02: Neutron Imaging of Advanced Combustion Technologies (Wissink)**
  - Direct “visual” experimental validation of model-predicted effects of solenoid armature bounce on non-linear injection characteristics with multiple injections has not been achieved – current validation data based on voltage/current waveforms and acoustical measurements
- **D.01.03: Evaporative Spray and Soot Film Combustion Modeling (Nguyen)**
  - Sensitivity in initial turbulence level and its influence in fuel jet spreading rate
  - Uncertainty in plume cone and plume direction angles
- **D.02.01: GDI Spray-Wall Interaction Modeling (Torelli)**
  - Sensitivity in initial turbulence level and its influence in fuel jet spreading rate
  - Uncertainty in plume cone and plume direction angles.
  - Uncertainty of experimental projected fuel mass away from the injector (> 5.0 mm)
- **D.02.02: Free Spray and Wall Impingement, Including VOF (Waters)**
  - Models are specifically tuned to different cases, potentially limiting predictibility
  - Evaporation model is based on single-particle evaporation, hence it needs a better model

Approach

- **Advantage of using free spray to understand wall impingement**
  - Validation with high quality experimental measurements within the PACE spray team to understand reliability of simulation results
  - How much of the total injected fuel will hit the wall as liquid ?
  - What is the composition of the liquid hitting the wall (need to understand preferential evaporation) ?
  - What is the effect of single (iso-octane) vs multi-component fuel (E00) ?
- **Multi-component injection method to address preferential evaporation**
  - Create a surrogate single-component liquid mixture. Can only evaporate into a single gaseous species.
  - Injected parcel consists of multiple components. Each liquid component can only evaporate into its respective gaseous species (e.g. liquid I-C8H18 -> gaseous I-C8H18). Capable of addressing preferential evaporation

E00 composition	
Species	% volume
IC8H18	46 %
NC5H12	36 %
NC11H24	18 %

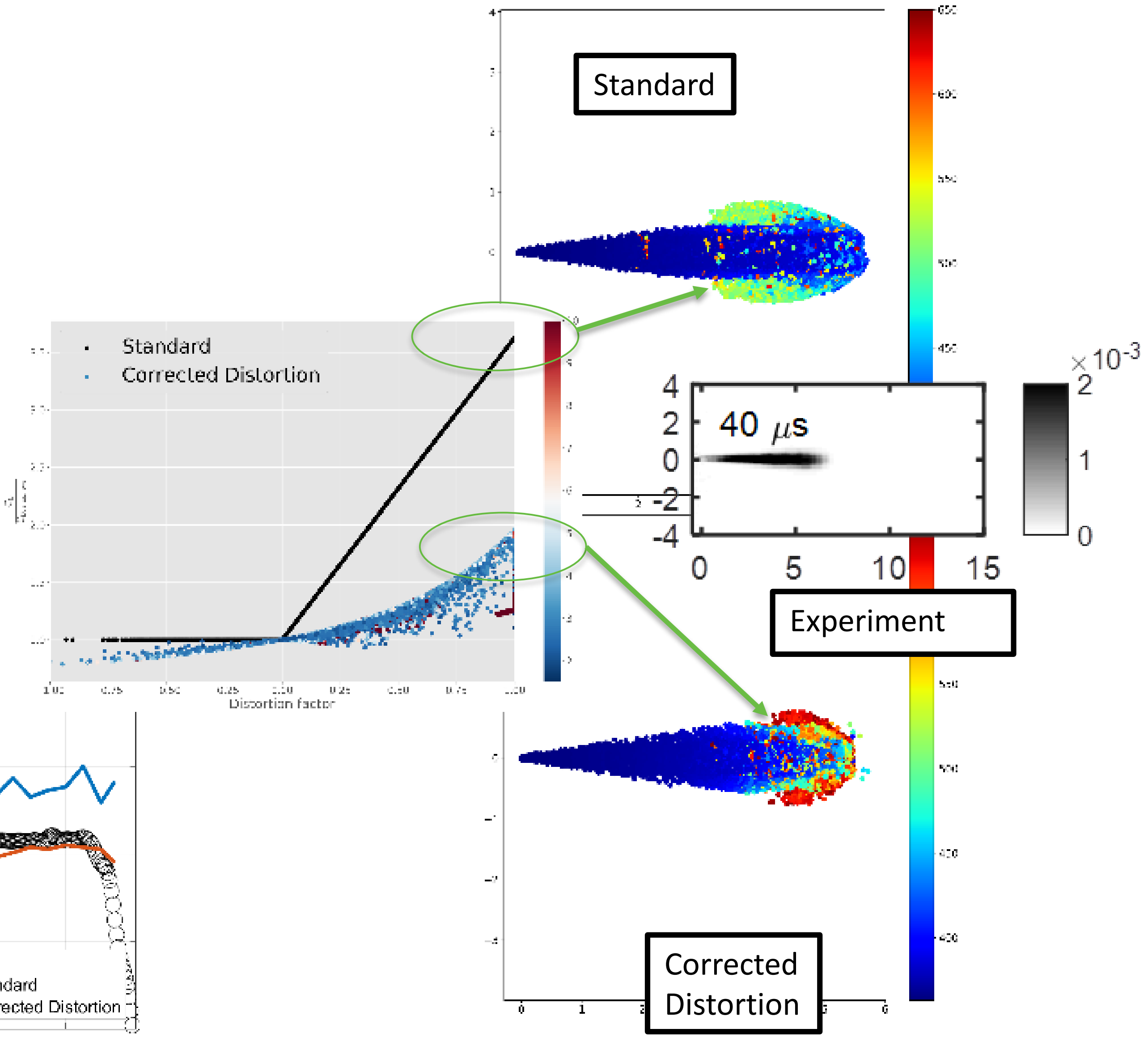
Numerical setup	
CFD code	CONVERGE v.2.4
Type of grid	AMR
Base grid	1.6 mm (SNL)
Minimum grid size	0.2 mm (SNL)

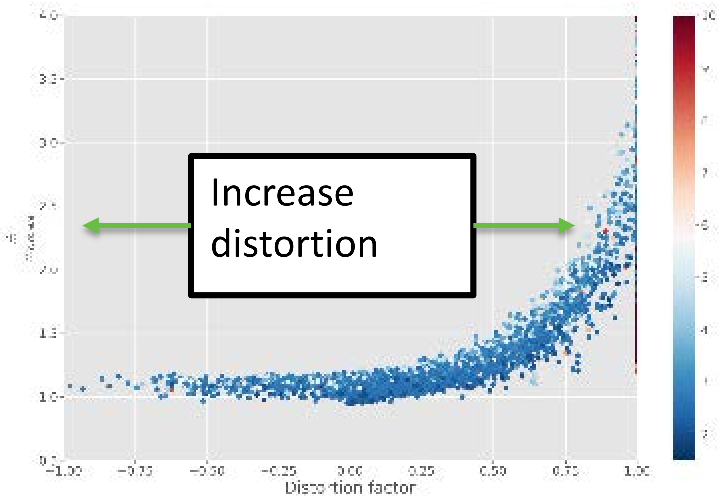
Models	
Turbulence	RANS $k-\varepsilon$ STD SNL
Spray model	Lagrangian parcel
Number of parcel injected	70,000 per nozzle
Break-up model	KH-RT
Vaporization	Corrected Distortion model
Droplet collision	No time counter (NTC)
Droplet drag	Corrected Distortion model
Droplet dispersion	O'Rourke
Injection Method	Blob

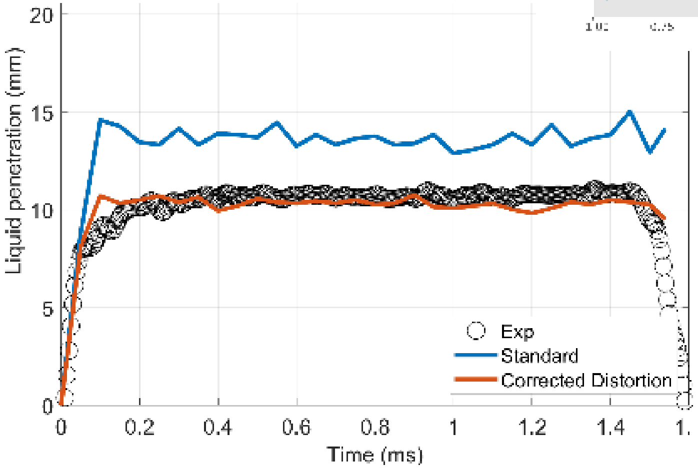
Case Name	Ambient condition
G3 hot	T=333 K, P=100 kPa
G3 cold	T=293 K, P=100 kPa

Accomplishments: more improvement in mixture formation for diesel spray

- **Lesson learned from diesel spray simulation (Spray A , T=900 K)**
  - For highly distorted drops, the Corrected Distortion model predict lower drop drag, eliminating unphysical droplet cloud behavior
  - Enhanced evaporation results in lower predicted liquid length that is in better agreement with experiments







Accomplishments: details on free-spray CFD simulations at Argonne

Details on the CFD code

- Software: **CONVERGE v3.0**
- Spatial discretization: second order
- Time discretization: first order with variable CFL based time-step (max 0.5 μs)

Mesh details

- Mesh base size: 4.0 mm
- Minimum mesh size: **0.125 mm** with fixed embedding near the injector tip and **0.250 mm** with AMR based on velocity, temperature and species gradients

Sub-model details

- Turbulence model: RANS RNG k-ε
- Liquid-gas coupling: Discrete Droplet Modeling (DDM)
- Injection model: Blob
- Break-up model: KHRT (B_1 = 10, C_{RT} = 0.5, shed factor = 0.10)
- Evaporation model: Frossling
- Collision model: OFF
- Drop drag model: Dynamic drop drag

Relevant initial and boundary conditions

- Initial turbulence : k = 0.0064 m^2/s^2, ε = 0.0508 m^2/s^3 (based on ECN database)
- Spray angles: experimental (@Sandia) average plume direction angle and time-varying cone angle

Technical Accomplishments and Progress D.02.02: (Waters)

KHRT break-up, collision, Vreman LES

10cm x 10cm x 10cm chamber with resolution of 2mm

- G1(T=530K, P=600kPa): Simulation is a little overshooting in the middle of

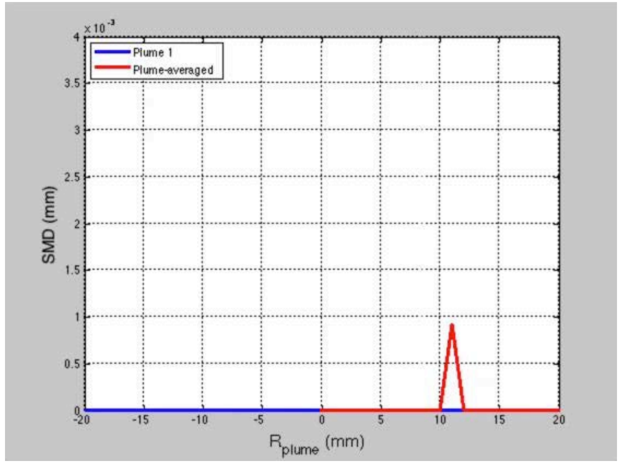
  time, and they match better later in time. (Fig.1)

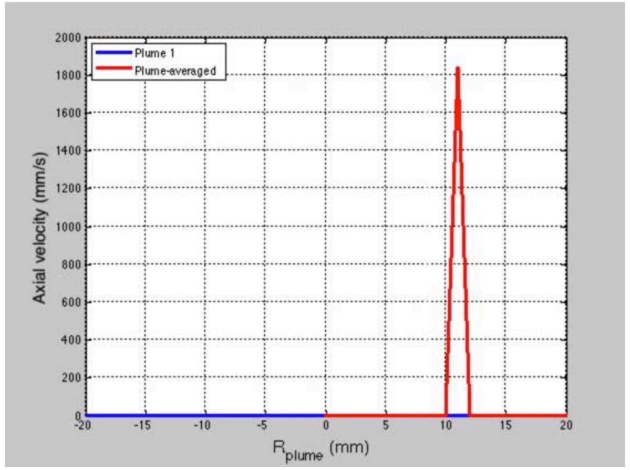
- Fig.2 shows the vapor and the particle at the end of injection time

Movies shows the SMD and axial velocity v.s. the plume radius at 15 mm from nozzle at different time:

SMD plume-averaged v.s. a plume at

Axial velocity plume-averaged v.s. a plume





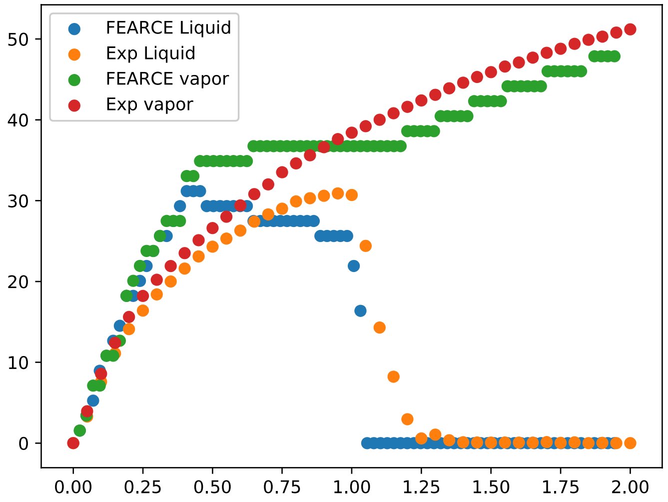


Fig. 1 Penetration plot

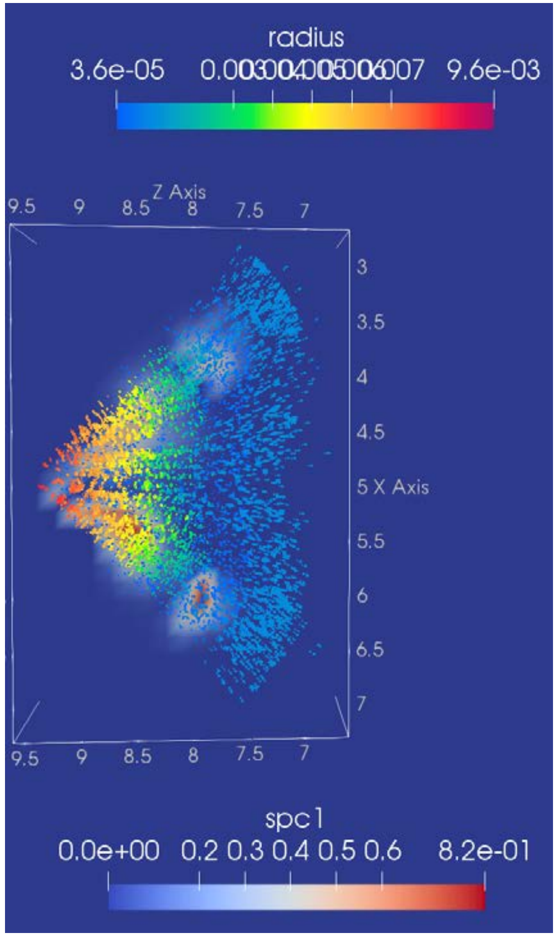


Fig.2 Particle (radius of particle in rainbow) and vapor (spc1) at t=6.7e-4 s